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Data Acquisition for Environmental Transport and Fate Screening for Compounds of Interest to the Office of Solid Waste

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DATA ACQUISITION FOR ENVIRONMENTAL TRANSPORT AND FATE SCREENING FOR COMPOUNDS OF INTEREST TO THE OFFICE OF SOLID WASTE

By

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16. ABSTRACT

Physical properties, equilibrium, and kinetic constants for evaluating the transformation and transport in aquatic systems for organic chemicals of interest to the US Environmental Protection Agency's Office of Solid Waste during FY 1983 have been obtained from the literature and calculated from theoretical or empirical relations. Values for selected physical properties such as melting point, boiling point, vapor pressure, water solubility, and octanol/water partitioning, and for rate constants such as hydrolysis, microbial degradation, photolysis, and oxidation are listed for each chemical along with the source of the data. Values are reported in units suitable for use in a current aquatic fate model. A discussion of the empirical relationships between water solubility, octanol/water partition coefficients, and partition coefficients for sediment and biota is presented.

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FOREWORD

The Exposure Assessment Group of EPA's Office of Research and Development has three main functions: 1) to conduct exposure assessments; 2) to review assessments and related documents; and 3) to develop guidelines for Agency exposure assessments. The activities under each of these functions are supported by and respond to the needs of the various EPA program offices. In relation to the first function, the Exposure Assessment Group sponsors projects for the purpose of gathering data used in exposure assessments. This study is one of those projects and was done for the Office of Solid Waste (OSW).

The Resource Conservation and Recovery Act of 1976 (RCRA) authorizes a regulatory program to identify those wastes which pose a substantial hazard to human health or the environment and to establish management standards sufficient to prevent such harm. A portion of this program focuses on individual chemicals and requires determining their toxicity, capacity to be transported to susceptible populations, and potential fate in the environment. The data compiled in this report are intended to assist OSW in predicting the probable fate and transport properties of compounds selected by OSW after study of various industrial waste streams.

James W. Falco, Director
Exposure Assessment Group

ABSTRACT

Physical properties, equilibrium, and kinetic constants for evaluating the transformation and transport in aquatic systems for organic chemicals of interest to the Environmental Protection Agency have been obtained from the literature and calculated from theoretical or empirical relations. Values for selected physical properties such as melting point, boiling point, vapor pressure, water solubility, and octanol/water partitioning, and for rate constants such as hydrolysis, microbial degradation, photolysis, and oxidation are listed for each chemical along with the source of the data. Values are reported in units suitable for use in a current aquatic fate model. A discussion of the empirical relationships between water solubility, octanol/water partition coefficients, and partition coefficients for sediment and biota is presented.

This report was submitted in partial fulfillment of Contract No. 68-03-2981 by SRI International under the sponsorship of the U.S. Environmental Protection Agency. This report covers a period from 1 May 1983 to 30 September 1983 and work reported herein was completed as of 30 September 1983.

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SECTION 1

INTRODUCTION

PURPOSE

Decisions on possible regulatory action or cost-effective remedial measures for toxic chemicals require an understanding of environmental and human risks associated with the manufacture, use, and disposal of chemicals. Part of the risk assessment requires the best scientific information about what the concentration of a chemical is in the environment. In the absence of reliable and extensive monitoring data, the concentration of a chemical can be estimated using one of several fate models and data for the individual processes that may be dominant for that chemical. These data may be measured in the laboratory, obtained from literature sources, or estimated using appropriate structure-activity relationships (SARs) or correlation methods. These data used with environmental parameters in a mathematical model constitute the process modeling approach (Baughman and Burns, 1980; Baughman and Lassiter, 1978; Smith et al., 1977; Mill, 1978).

The compounds listed in this report were of concern to the Office of Solid Waste after study of waste streams from certain industrial processes. Others are recognized by-products or potential trace by-products which might have substantial health impacts if appropriate waste disposal practices are not followed. The Office of Solid Waste has requested that chemical-specific Health and Environmental Effects Profiles, or preliminary risk assessments, be prepared from existing literature sources to assist in deciding whether the chemical should be listed as hazardous wastes under provisions of the Resource Conservation Act and Recovery Act of 1976, Section 3001. The Office of Health and Environmental Assessment, consequently is examining the toxicological, environmental and chemical literature as background for this work. This report compiles literature data or estimates for 10 fundamental physical and chemical parameters for 74 chemicals which subsequently will be analyzed to predict their potential environmental transport, fate and persistence.

These data are to be used to decide what chemicals clearly would not persist in aquatic environments because of exceptional reactivity and what environments may be of particular concern because of dominant volatilization or sorption processes. This information will also be used to decide what data gaps exist and what particular process data need to be obtained for subsequent and more detailed assessments.

The data are made available in this report with the expectation that they may be of interest in other assessment efforts. Use of the data in the context of other assessments requires that each user understand the sources and limitations of the data. Each user must decide what additional data are required for the particular assessment. Any user of these data must particularly recognize that some values were estimated by SRI staff with expertise in the process of interest, and that considerable subjective judgment was applied for some of the estimates. Such judgments based on even crude analogies are indeed valuable and acceptable in screening level evaluations. In cases where even expert judgment cannot be used to provide a value, no value was entered. Users of these data are encouraged to conduct more intensive literature searches or to consult other knowledgeable scientists to augment or supplant data in this report.

In this report, "process data" are defined as data relating to rate constants, equilibrium constants, or physical properties that describe the intrinsic processes the chemicals may undergo independent of environmental influences. "Environmental parameter" in this report refers to properties or data that describe (or are a function of) the environment.

BACKGROUND

The processes that can be important for transforming or transporting a chemical in an aquatic environment are shown in Figure 1.1. The following discussion summarizes the mathematical basis for the process modeling approach applied to aquatic systems: (1) the evaluation of rates of loss of chemical due to transformations and volatilization processes, (2) the influence of sorption processes on the rates of loss of chemical, and (3) the prediction of concentration and half-life of chemical in the aquatic environment, including terms for input of chemical, dilution, and flow out of the environment. This discussion assumes that sorption to particulates in the environment is not kinetically controlled (i.e., sorption equilibrium is attained instantaneously).

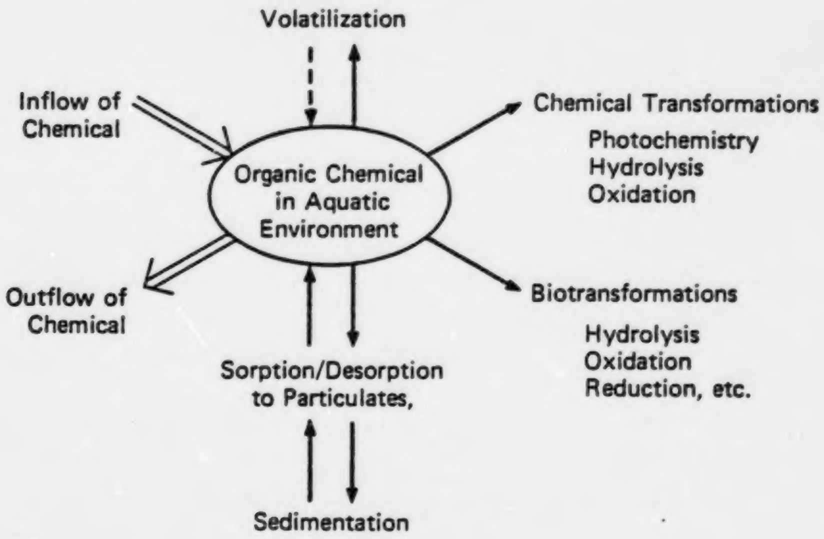

Volatilization
Inflow of Chemical
Chemical Transformations
Photochemistry
Hydrolysis
Oxidation
Organic Chemical in Aquatic Environment
Outflow of Chemical
Biotransformations
Hydrolysis
Oxidation
Reduction, etc.
Sorption/Desorption to Particulates,
Sedimentation

FIGURE 1.1 TRANSPORT AND TRANSFORMATION PROCESSES IN AQUATIC ENVIRONMENTS

EVALUATION OF CHEMICAL LOSS RATES

The rate of loss of a chemical due to the above transformation processes and volatilization, R_T, is given by the sum of the rates of the individual processes, R_i, according to the equation

$$R_T = \Sigma R_i = \Sigma k_i'[E_i][C] \tag{1.1}$$

where k_i' is the rate constant for the i-th process, $[E_i]$ is an environmental parameter that is kinetically important for the i-th process, and [C] is the concentration of the chemical. The calculations of R_i for individual processes from environmental parameter and process data are discussed in subsequent sections. The important environmental parameters for each process have been reviewed, and the use of the parameters in the calculations of environmental transformation rates has been discussed in detail by Baughman and Burns (1980), Mill (1978), and Smith et al. (1977).

The above expression for R_T assumes that the loss of chemical is first order in the chemical concentration, as certainly must be the case at the highly dilute concentrations expected in the environment. Equation (1.1) also requires that the rate of loss of chemical due to any one process R_i is first order in the environmental parameter term E_i; R_i is then considered as following overall second-order kinetic behavior. If it is assumed that the low concentration of chemical in the environment has no significant effect on the environment (for example, does not change pH, biomass, dissolved oxygen, etc.) and that the environmental parameter, E_i, is constant over a specific region and time period, the term k_i' $[E_i]$ can be expressed as a simple pseudo-first-order rate constant, k_i, and then

$$R_T = [\Sigma k_i][C] = k_T[C] \tag{1.2}$$

or

$$k_T = \Sigma k_i \tag{1.3}$$

where k_T is the overall pseudo-first-order rate constant for loss of chemical due to transformation and volatilization. The half-life for loss of chemical due to these processes is then given by

$$t_{1/2} = \ln 2/k_T \qquad (1.4)$$

INFLUENCE OF SORPTION

In addition to losses of chemicals due to these transformation and volatilization processes, sorption to particulates can also reduce the concentrations of chemicals in aquatic systems. These particulates may be either suspended sediments or biotic in origin and the particulates may eventually be deposited into benthic sediments. The suspended or benthic sediment may later serve as a source of chemical from sorption-desorption equilibrium as the chemical in solution volatilizes or undergoes transformation in the water column. If biotransformation does not occur in biota (such as bacteria, algae, and fish), the chemical may be released back into solution when the organism dies and decomposes. The understanding of chemical transformation when the chemical is sorbed onto particulates is inadequate to predict or measure the rates of such reactions for use in modeling. Therefore, the following discussion assumes that no transformations occur on particulates and that sorption is completely reversible and rapid in comparison with transformations that occur in solution.

The partitioning of a chemical between particulates (sediment or biota) and water at the low concentrations of chemicals usually found in the environment can be expressed as a partition coefficient K_p:

$$K_p = C_s/C_w \qquad (1.5)$$

where C_s and C_w are the equilibrium concentrations of chemical on sediment and in water, respectively (Baughman and Lassiter, 1978; Smith and Bomberger, 1982).

By convention, K_p is unitless when C_s is in units that are equivalent to C_w (i.e., C_s is in g chemical/g particulate and C_w is in g chemical/g water). In this discussion, $[C_w]$ will be defined in these weight units and $[C]$ will be defined in molecular units (moles L^{-1});

because 1 g water is approximately 1 mL, it follows that $[C] = 10^3[C_w][MW]^{-1}$ where MW is the molecular weight of chemical. Note that [C] and $[C_w]$ can be used interchangeably in expressions such as equation (1.2) because first-order rate constants are concentration independent, but the rate of loss term, R, is of course defined in units corresponding to $[C_w]$ or [C].

For a chemical in aqueous solution containing particulates, the chemical is equilibrated between the water and particulate P according to the relation

$$C + P \rightleftharpoons C\text{-}P \qquad (1.6)$$

and the partition coefficient can be rewritten as

$$K_p = \frac{[C\text{-}P]}{[C_w][P]} \qquad (1.7)$$

where [C-P] is the mass of sorbed chemical per unit solution volume and [P] is the mass of sorbing particulate per unit solution volume. The mass balance of chemical in the solution-sediment system is given by

$$[C_T] = [C\text{-}P] + [C_w] \qquad (1.8)$$

where $[C_T]$ is the total mass of chemical in a unit solution volume of water containing [P] grams of particulate. Combining equations (1.7) and (1.8) then gives the fraction of the total chemical dissolved in solution:

$$\frac{[C_w]}{[C_T]} = \frac{1}{K_p[P] + 1} \qquad (1.9)$$

Baughman and Lassiter (1978) have pointed out that, given the relationship shown in equation (1.9), the fraction of chemical in solution may be quite high in spite of a large K_p value because the sediment or biota loading, [P], is often low in aquatic systems (i.e., $K_p[P] < 1$).

The concentration of chemical in solution $[C_w]$ in the presence of a particulate-water system is then given by

$$[C_w] = \frac{[C_T]}{[P]K_p + 1} \qquad (1.10)$$

Substituting equation (1.10) into equation (1.2) for the rate of loss of chemical then gives

$$R_T = \frac{k_T C_T}{[P]K_p + 1} \qquad (1.11)$$

This relationship shows that unless transformation on particulate is as fast as or faster than that in solution, the net effect of sorption will be to reduce the overall rate of loss of chemical from the aquatic system. From equation (1.11), it also follows that the half-life of the chemical is given by

$$t_{1/2} = \frac{([P]K_p + 1)\ln 2}{k_T} \qquad (1.12)$$

The process modeling approach is then a valuable tool in risk assessments. Although values of $t_{1/2}$ or C_w can be manually calculated, the calculations are more easily done using computer programs. One such computer model is EXAMS, which allows the user to choose environmental parameters and is able to accommodate chemicals when several processes compete to be the important fate pathway. Computer models also allow for sophisticated and environmentally realistic dynamic models to be used rather than assuming steady-state conditions.

REFERENCES

Baughman, G. L., and L. A. Burns. 1980. Transport and Transformation of Chemicals: A Perspective. In: The Handbook of Environmental Chemistry, Vol. 2, Part A. O. Hutzinger, Ed. Springer-Verlag, New York.

Baughman, G. L., and R. R. Lassiter. 1978. Prediction of Environmental Pollutant Concentration. In: Estimating the Hazard of Chemical Substances to Aquatic Life. ASTM STP 657. J. Cairns, Jr., K. L. Dickson, and A. W. Maki, Eds. American Society for Testing and Materials, Philadelphia, PA.

Mill, T. 1978. Data Needed to Predict Environmental Fate of Organic Compounds. Symposium on Environmental Fate held at American Chemical Society Meeting, Miami, FL, September 1978.

Smith, J. H., and D. C. Bomberger. 1982. Volatilization from Water. In: Laboratory Protocols for Evaluating the Fate of Organic Chemicals in Air and Water. EPA-600/3-82-022. U.S. EPA, Washington, DC.

Smith, J. H., W. R. Mabey, N. Bohonos, B. R. Holt, S. S. Lee, T.-W. Chou, D. C. Bomberger, and T. Mill. 1977. Environmental Pathways of Selected Chemicals in Freshwater Systems. Part I. Background and Experimental Procedures. EPA-600/7-77-113. U.S. EPA, Washington, DC.

SECTION 2

DEFINITIONS OF PROCESSES AND SOURCES OF DATA

BASIS FOR DERIVATION OF DATA

The data on chemicals given in this report were obtained from the literature and from calculations based on theory, SARs, or empirical calculations. In general, the physical properties of a chemical are functions of the molecular structure as an entity; that is, the elemental composition, spatial relationships and size, molecular weight, and functional groups of the molecule all may contribute to the property of the chemical. In contrast, the chemical or biological reactivity of a molecule is usually caused by selected functional groups in the molecular structure, and the functional group may undergo transformation with sometimes only minor changes in the total structure of the molecule.

The individual processes that chemicals may undergo can then be classified and evaluated according to specific physical properties or the reactive functional groups that these chemicals may have in common. The basis for the empirical correlations between K_{ow} and S_w is discussed in Section 4. These constants describe equilibrium processes for the chemical between water and a second (organic) phase. Similarly, the volatilization of a chemical can be evaluated in terms of Henry's constants, which are functions of vapor pressure and water solubility.

The reactivity of a chemical can be classified according to select functional groups in the molecular structure. For evaluations of hydrolysis reactions, chemicals are classified as carboxylic acid esters ($-CO_2R$), carboxylic acid amides ($-CONH_2$), alkyl halides (R-X), and phosphoric acid esters ($(RO)_3PO$), to name only a few. Data for hydrolysis of a chemical can often be estimated by analogy to another chemical with a similar functional group or calculated by more formal procedures using linear free-energy relationships such as the Taft equation, the Hammett equation, or other such correlations (Mill, 1979; Wolfe et al., 1978 and 1980).

Chemical oxidation rate constants can be calculated by evaluating the reaction of an oxidant at a particular type of carbon-hydrogen bond (i.e., hydrogen abstraction process) or at an olefinic bond. No SAR or correlation method is available for predicting a direct photolysis rate constant except by analogy to other chemicals, which is often unreliable because of the complex chemistry of photoexcited states.

For this report, data obtained from calculations involving theory, SARs, or empirical correlations have been clearly identified so that the user can recognize the source of such data and can recalculate data using current or improved procedures.

The following briefly describes the environmental processes and the process data important in aquatic fate assessments. The process data are discussed in the order that they appear on the data sheets. The sources of the process data are also discussed.

CHEMICAL NAME, CHEMICAL ABSTRACTS SERVICE REGISTRY NUMBER, AND MOLECULAR WEIGHT

The names of the chemicals used on the data sheets are those as given on the original EPA list. The Chemical Abstracts Service (CAS) number has been obtained mainly from the original EPA list. Handbooks, catalogs, or the CAS were used when necessary. The molecular weight (MW) has been calculated from the molecular formula. Although the MW is not used for environmental assessments, it is required for conversion of units from ppm to molar units (M). The MW has also been used to calculate the molecular weight/oxygen ratio.

WATER SOLUBILITY

Water solubility (S_w) data are required for calculating Henry's constant and for calculating other partition coefficients using the correlation equations discussed in Section 4. Values of S_w (ppm or mg L^{-1}) were calculated from K_{ow} using a correlation equation developed by Yalkowsky and Valvani (1980).

For organic pollutants that are liquid in their pure state at 25°C

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW \qquad (2.1)$$

where MW is the molecular weight of the pollutant (g $mole^{-1}$). For organic pollutants that are solid in their pure state at 25°C

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW - (\frac{\Delta S_F}{1360})(mp - 25) \qquad (2.2)$$

where mp is the melting point of the pollutant (°C) and ΔS_F is the entropy of fusion of the pollutant (cal $mol^{-1}deg^{-1}$). If ΔS_F is not known, it may be approximated by

$$\Delta S_F \sim 13.6 + 2.5 (n - 5) \qquad (2.3)$$

where n is the number of flexible atoms (i.e., atoms not involved in double bonds, triple bonds, or part of a ring structure) in the pollutant molecule, other than hydrogen. If n is less than 5, n - 5 is set equal to zero.

For solids that had no literature melting points available, S_w was calculated using the equation for liquids. This results in a maximum S_w and should be used only for a screening risk assessment.

MELTING AND BOILING POINT

These data are not used directly in aquatic fate assessments, but they show in which phase (gas, liquid, solid) the pure chemical is found under environmental conditions. Boiling point data are cited for 760 torr (1 atmosphere) unless otherwise noted. The melting point should be used in the calculation of water solubility from octanol/water partition coefficient (K_{ow}) data for compounds that are solids above 25°C.

VAPOR PRESSURE

The vapor pressure P_v (torr) of an organic chemical is, in itself, a qualitative or relative measure of the volatility of the chemical in its pure state and can be used to calculate the Henry's constant used in volatilization rate constant calculations. Unless otherwise specified, the P_v values listed are at 25°C.

Vapor pressure data not found in the literature were calculated using procedures described by Grain (1982). The method uses a modification of the Watson correlation to express the temperature dependence of ΔH_v such that

$$\Delta H_v \approx \Delta H_{vb} [3 - 2(T/T_B)]^m \quad (2.4)$$

where ΔH_v is the heat of vaporization at temperature T, ΔH_{vb} is the heat of vaporization at the normal boiling point, and m is a constant that depends upon the physical state. Substitution in the Clausius-Clapeyron equation and integration results in an expression with adjustable parameters that depend on the molecular structure, functional groups, and physical state at the temperature of interest. With further modification, the method can also be used to extrapolate vapor pressures from one temperature to another.

This procedure has an estimated maximum error of 7.1% over the pressure range 10-760 torr, 50% over 10^{-3}-10 torr, and 200% below 10^{-3} torr. The average error is <50%, which is often less than the range of P_vs found in the literature.

MOLECULAR WEIGHT TO OXYGEN RATIO

The molecular weight to oxygen ratio is used to estimate the volatilization rate constant for a chemical (Mabey et al. 1983). The ratio was calculated from the molecular weights of the chemical and molecular oxygen (the latter is 32 g/mole).

OCTANOL/WATER PARTITION COEFFICIENT

The octanol/water partition coefficient K_{ow} has been used in medical and environmental science as a measure of the hydrophobicity/hydrophilicity of chemicals (Hansch and Leo, 1979; Kenaga and Goring, 1978). The K_{ow} values in this report were used to calculate S_w; K_{ow} values also are useful for estimating sediment and biota partitioning coefficients (see Section 4). The calculation of K_{ow} from structural features of the molecule is also discussed in Section 4.

HYDROLYSIS RATE CONSTANTS

Hydrolysis refers to reaction of a chemical with water, usually resulting in the introduction of a hydroxyl function into a molecule and loss of a leaving group -X:

$$R\text{-}X + H_2O \longrightarrow ROH + HX \tag{2.5}$$

The hydrolyses of some classes of compounds are catalyzed by acid or base, and therefore the hydrolysis rates of these chemicals in the environment can be pH dependent. The subject of hydrolysis in aquatic systems has been reviewed in detail by Mill et al. (1982), and an extensive compilation of hydrolysis data was published in a review by Mabey and Mill (1978).

The rate of hydrolysis of a compound at a specific pH value is given by the equation

$$R_H = k_h[C] = (k_A[H^+] + k_N + k_B[OH^-])[C] \tag{2.6}$$

where k_h is the first-order rate constant for hydrolysis at the pH, k_A and k_B are second-order rate constants for acid- and base-promoted hydrolyses respectively, and k_N is the first-order rate constant for the pH-independent, neutral hydrolysis process. Using the autoprotolysis equilibrium expression

$$[H^+][OH^-] = K_w \tag{2.7}$$

equation (2.6) can be rewritten as

$$k_h = k_A[H^+] + k_N + \frac{k_B K_w}{[H^+]} \tag{2.8}$$

Equation (2.8) shows that k_h will depend on the pH of the aquatic system and on the relative values of k_A, k_B, and k_N. At present, no reliable information shows that hydrolysis rates in aquatic environments will be catalyzed by species other than $[H^+]$ or $[OH^-]$.

The hydrolysis rate constants k_A, k_B, and k_N used to calculate k_h as a function of pH are described below along with the source codes for calculating or estimating the values of the rate constants.

ACID-PROMOTED HYDROLYSIS RATE CONSTANT

The acid-promoted hydrolysis rate constant k_A ($M^{-1}h^{-1}$) is for the acid-promoted hydrolysis of a chemical. In regions where only k_A contributes to hydrolysis (i.e., $k_A[H^+] >> k_N = k_B[OH^-]$), k_h will decrease by a factor of 10 for each 1-unit increase in pH.

BASE-PROMOTED HYDROLYSIS RATE CONSTANT.

The base-promoted hydrolysis rate constant k_B ($M^{-1}h^{-1}$) is for the base-promoted (OH^-) hydrolysis of a chemical. In regions where only k_B contributes to hydrolysis, k_h will increase by a factor of 10 for each 1-unit increase in pH.

NEUTRAL-HYDROLYSIS RATE CONSTANT.

The neutral-hydrolysis rate constant k_N (h^{-1}) is for the pH-independent hydrolysis of a chemical. Data or sources pertaining to the hydrolysis of the organic chemicals have been entered in the data sheets in several ways. When a chemical structure had no hydrolyzable functional groups, NHFG was entered. When chemical hydrolysis occurs only at extreme pH values or temperatures or with catalysts not available in aquatic environments, HNES was entered (hydrolysis not environmentally significant). Other data for hydrolysis are referenced or are based on analogy to similar chemicals.

MICROBIAL DEGRADATION RATE CONSTANT

Biotransformations are undoubtedly important processes for degradation of chemicals in aquatic environments, resulting in hydrolysis, oxidation, and reduction of the chemical structure to ultimately produce carbon dioxide and water. The complex factors influencing the biotransformation of a chemical include pH, temperature, dissolved oxygen, available nutrients, other organic chemicals (synthetic or naturally occurring) that may serve as cometabolites or alternative energy sources, and the populations and types of organisms capable of transforming the chemical. For most assessments, the initial biotransformation step is of prime importance (i.e., removal of the specific chemical from the environment). However, the biotransformation process is still too complex to be used to reliably predict a biotransformation rate constant using theoretical approaches such as those available for chemical and physical processes.

Maki et al. (1980) recently reviewed some of the aspects of the measurement of biotransformation rates and the use of such data. The rates of biotransformation are complex functions of chemical concentration and microbial biomass. However, at the typical concentrations of a chemical in the environment (< 1 ppm), the rates may be expected to follow second-order kinetics because they are first order in chemical kinetics and first order in biomass kinetics. Furthermore, the microorganism growth due to consumption of the chemical may not be significant; therefore, the rates of biotransformation are pseudo-first-order as a function of the chemical concentration.

The biotransformation data given in this report were estimated for the approach described by Baughman et al. (1980), in which the rate of biotransformation of a chemical, R_B, is given by the expression

$$R_B = - k_b[B][C] \tag{2.9}$$

where k_b is a second-order rate constant for biotransformation of a chemical by bacteria of population [B] in the solution phase of the water column. When k_b is given in mL cell^{-1} h^{-1}, the units of [B] are in cell mL^{-1}. Because data for k_b were not available for most chemicals covered by this report, the rate constants were estimated solely for use in aquatic fate modeling by EPA. These data were estimated using on relative rates of biodegradation of the chemicals as reported in literature, structural analogies, and judgment of SRI staff with expertise in biotransformation studies. These data have been estimated and appropriate caution should be exercised in the use of the data.

PHOTOLYSIS RATE CONSTANT

The direct photolysis rate constants k_p (h^{-1}) for most of the chemicals cannot be estimated because of insufficient spectral and quantum yield data. For chemicals where no light absorption occurs above the solar cutoff (300 nm), the rate constant can be considered as zero, and therefore photolysis is not environmentally relevant (NER).

In cases where the chemical is expected to photolyze in the environment but no data are available, no value is entered. Similarly, no value is entered if nothing is known about a chemical's photolytic reactivity. No data for indirect photolysis of chemicals is provided in this report except that which results from oxidation processes (see next section).

OXIDATION RATE CONSTANTS

Chemical oxidation of organic chemicals in aquatic environments may be caused by several different oxidants, among which are singlet oxygen ($^1O_2$), alkyl peroxyl radical ($RO_2\cdot$), alkoxy radical ($RO\cdot$), or hydroxyl radical ($\cdot OH$). The source of these oxidants is primarily photochemical, but because the oxidants react with chemicals in their ground state, and oxidation therefore does not involve the photochemistry of the chemical itself, oxidations are reasonably considered as discrete processes apart from photochemistry. Each oxidant has a unique reactivity toward organic moieties, and the relative and absolute concentrations of these oxidants will vary with environmental parameters, such as concentration and origin of humic-fulvic materials and sunlight intensity.

Literature information classifies reported data on oxidation of organic chemicals by oxy radicals such as $RO_2\cdot$ and $^1O_2$. The laboratory study conducted by Mill et al. (1982) using natural waters indicates that $RO_2\cdot$ radical concentrations of $\sim 1 \times 10^{-9}$ M may be present in the surface waters of sunlit water bodies. Oxidation reactions initiated by $RO_2\cdot$ include the following:

$$RO_2\cdot + -C\text{-}H \longrightarrow RO_2H + -C\cdot \qquad (2.10)$$

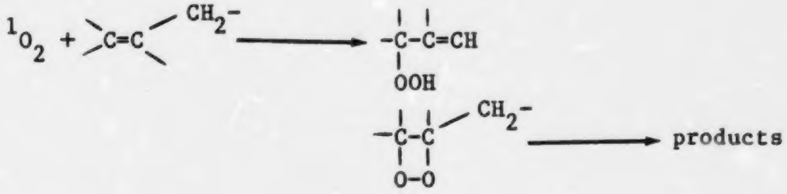
$$RO_2\cdot + C{=}C \longrightarrow RO_2\text{-}C\text{-}C\cdot \qquad (2.11)$$

$$RO_2\cdot + ArOH \longrightarrow RO_2H + ArO\cdot \qquad (2.12)$$

$$RO_2\cdot + ArNH_2 \longrightarrow RO_2H + Ar\dot{N}H \qquad (2.13)$$

Of these reactions, the last two are quite rapid in aquatic environments ($t_{1/2}$ < several days), whereas the others are slower and usually will not be important for most chemicals.

Zepp et al. (1978) have shown that $^1O_2$ can be formed at $\approx 1 \times 10^{-12}$ M concentrations in sunlit natural waters. The most important reactions for $^1O_2$ with organic chemicals are those involving reaction with olefinic moieties (Ranby and Rabek, 1978).



(2.14)

Some rate constants for $^1O_2$ and $RO_2\cdot$ are listed in a review by Mill (1980).

The rate of loss of organic chemicals R_{OX} by oxidation is

$$R_{OX} = k_{RO_2\cdot}[RO_2\cdot][C] + k_{^1O_2}[^1O_2][C] + k_{OX}[OX][C] \qquad (2.15)$$

where k_{OX} and [OX] are the rate constants and concentration values for other unspecified oxidants. Only data for the second-order rate constants $k_{RO_2\cdot}$ and $k_{^1O_2}$ have been estimated for this report. When two rate constants are given on the data sheets, the second-order rate constants should be multiplied by their respective oxidant concentrations to determine which of the first-order rate constant values is larger, and that rate constant should be used for an assessment.

Apart from a direct measurement of a rate constant at a specific temperature (which is rare), most rate constants in this report were obtained either from extrapolation of a rate constant for the organic chemical measured at another temperature or from a correlation of structure with reactivity as discussed below.

RATE CONSTANT FOR OXIDATION BY ALKYL PEROXYL RADICAL

Because many chemicals on the list of chemicals of concern have several kinds of reactive centers for oxidation by $RO_2\cdot$, the overall rate constant k_{RO_2} $(M^{-1}h^{-1})$was obtained by first calculating the individual rate constants for each reactive site and then summing these rate constants. For example, acrolein has two reactive sites: (1) addition to the double bond and (2) H-atom transfer from the carbonyl

$$RO_2\cdot + CH_2{=}CHCHO \xrightarrow{k_1} RO_2C{-}\dot{C}{-}CHO \qquad (2.16)$$

$$RO_2\cdot + CH_2{=}CHCHO \xrightarrow{k_2} CH_2{=}CH\dot{C}O + RO_2H \qquad (2.17)$$

$$k_{RO_2} = k_1 + k_2 \qquad (2.18)$$

When one oxidation process was found to be fast, the important oxidant was listed and the other reactions were ignored. When there were more than one -CH bond of a given kind, the rate constant was multiplied by the number of similar -CH bonds to give the correct total rate constant for oxidation of that CH-bond.

Two procedures were used to calculate individual k_{OX} values for $RO_2\cdot$ reactions. In the first, when a structure was analogous to another chemical structure with a measured rate constant at a similar temperature, the measured rate constant was used directly (Hendry et al., 1974). (The -CHO bond in acrolein is an example.) The second procedure, used most often, is based on SARS established by Howard and coworkers for H-atom transfer (Korcek et al., 1972) and addition to double bonds (Howard, 1972), as shown below.

For the H-atom transfer reaction

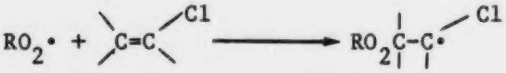
$$\log k_{RO_2} = 18.96 - 0.2[D(R{-}H)] \qquad (2.19)$$

where D(R-H) is the bond dissociation energy of the CH-bond.

For the RO_2 addition to double bonds

$$\log k_{RO_2} = [16.54 - 0.2D(XCR_2\text{-}H)]/0.75 \qquad (2.20)$$

where $D(XCR_2\text{-}H)$ is the bond dissociation energy of a species that gives the radical formed by RO_2 addition and where RO_2 is assumed to have the same effect as methyl (Me) on D(C-H). Thus for oxidation of vinyl chloride



(2.21)

the closest analog would be $MeCH_2\dot{C}HCl$, and the value of $D(MeCH_2CHCl\text{-}H)$ would be used in equation (2.20). Bond dissociation energies were taken from Furuyama et al. (1969).

RATE CONSTANT FOR OXIDATION BY SINGLET OXYGEN

Only a few of the chemicals tabulated in this report are reactive toward $^1O_2$; these include some polycyclic aromatic and a few olefinic double bond or diene systems. All reactive chemicals were assigned rate constants by analogy with similar structures that have shown rate constants for reaction with singlet oxygen. For cyclic olefins, the values of Matsuura et al. (1973) were used. For alicyclic olefins and other structures, the rate data summarized by Gollnick (1978) were used.

REFERENCES

Baughman, G. L., D. L. Paris, and W. C. Steen. 1980. Quantitative Expression of Biotransformation Rate. In: Biotransformation and Fate of Chemicals in Aquatic Environments. A. W. Maki, K. L. Dickson, and J. Cairns, Jr., Eds. American Society for Microbiology, Washington, DC.

Furuyama, S., D. M. Golden, and S. W. Benson. 1969. J. Am. Chem. Soc. 91, 7564-7569.

Göllnick, K. 1978. In: Singlet Oxygen. B. Ranby and J. F. Rabek, Eds. John Wiley and Sons, New York.

Grain, C. 1982. Vapor Pressure. In: Handbook of Chemical Property Estimation Methods. W. J. Lyman, W. F. Reehl, D. H. Rosenblatt, Eds. McGraw-Hill Book Company, New York.

Hansch, C., and A. Leo. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. Wiley-Interscience. New York.

Hendry, D. G., T. Mill, L. Piszkiewicz, J. A. Howard, and H. K. Eigenmann. 1974. J. Phys. Chem. Ref. Data. 3, 937-978.

Howard, J. A. 1972. Adv. Free Radical Chem. 4, 49-174.

Kenaga, E. E., and C. A. I. Goring. 1978. Relationship Between Water Solubility, Soil-Sorption, Octanol/Water Partitioning, and Bioconcentration of Chemicals in Biota. In: Aquatic Toxicology, ASTM STP 707, J. G. Eaton, P. R. Parrish, and A. C. Hendricks, Eds. American Society for Testing and Materials, Philadelphia, PA.

Korcek, S., J. H. B. Chenier, J. A. Howard, and K. U. Ingold. 1972. Can. J. Chem. 50, 2285-2297.

Mabey, W. R., and T. Mill. 1978. J. Phys. Chem. Ref. Data. 7, No. 2, 383-415.

Mabey, W. R., T. Mill, and R. T. Podoll. 1983. Estimation Methods for Process Constants and Properties Used in Fate Assessments. Final Report for Work Assignment No. 5 in partial fulfillment of EPA Contract No. 68-03-2981, U.S. EPA, Athens, GA.

Maki, A. W., K. L. Dickson, and J. Cairns, Jr., Eds. 1980. Biotransformation and Fate of Chemicals in Aquatic Environments. American Society for Microbiology, Washington, DC.

Matsuura, T., A. Horinaka, and R. Nakashima. 1973. Chem. Lett. 887-890.

Mill, T. 1979. Structure Reactivity Correlations for Environmental Reactions. EPA-560/11-79-012. U.S. EPA, Washington, DC.

REFERENCES

Mill, T. 1980. Photooxidation in the Environment. In: The Handbook of Environmental Chemistry, Vol. 2, Part A. O. Hutzinger, Ed. Springer-Verlag, New York.

Mill, T., W. R. Mabey, and D. G. Hendry. 1982. Hydrolysis in Water. In: Laboratory Protocols for Evaluating the Fate of Organic Chemicals in Air and Water. EPA-600/3-82-022. U.S. EPA, Washington.

Ranby, B., and J. F. Rabek, Eds. 1978. Singlet Oxygen. John Wiley and Sons, New York.

Wolfe, N. L., L. A. Burns, and W. C. Steen. 1980. Chemosphere. 9, 393-402.

Wolfe, N. L., R. G. Zepp, and D. F. Paris. 1978. Water Res. 12, 561-563.

Yalkowsky, S. H., and S. C. Valvani. 1980. J. Pharm. Sci. 69, No. 8, 912-922.

Zepp, R. G., N. L. Wolfe, G. L. Baughman, and R. C. Hollis. 1978. Nature. 267, 421-423.

SECTION 3

DATA SHEETS FOR CHEMICALS OF INTEREST

This section contains a list of data sheets showing the Chemical Abstract Services registry number and compound name, a list of source codes for the data sheets, and the data sheets and references for this work assignment.

LIST OF DATA SHEETS

Number	CAS Registry Number	Compound Name
1	102-36-6	3,4-Dichlorophenylisocyanate
2	102-82-9	Tributylamine
3	314-40-9	Bromacil
4	330-55-2	Linuron
5	624-92-0	Dimethyldisulfide (2,3-Dithiabutane)
6	110-81-6	Diethyldisulfide (3,4-Dithiahexane)
7	30453-31-7	Ethylpropyldisulfide (3,4-Dithiaheptane)
8	68-85-0	Benzoic acid
9	93-58-3	Methylbenzoate
10	99-04-7	3-Methylbenzoic acid
11	99-94-3	4-Methylbenzoate
12	619-21-6	3-Formylbenzoic acid
13	619-66-9	4-Formylbenzoic acid
14	88-99-3	Phthalic acid
15	100-21-0	Terephthalic acid
16	120-61-6	Dimethylterephthalate
17	1679-64-7	Methylterephthalate
18	121-91-5	Isophthalic acid
19	528-44-9	Trimellitic acid (1,2,4-Benzenetricarboxylic acid)
20	2303-16-4	Diallate
21	2303-17-5	Triallate
22	12427-38-2	Maneb
23	1134-23-2	Cycloate
24	1929-77-7	Vernolate
25	1114-71-2	Pebulate
26	2212-67-1	Molinate
27	2008-41-5	Butylate
28	1563-66-2	Carbofuran
29	63-25-2	Carbaryl
30	39076-02-3	sec-Butylcarbamic acid, methyl ester

LIST OF DATA SHEETS (continued)

Number	CAS Registry Number	Compound Name
31	148-18-5	Dithiocarbamate
32	8018-01-7	Mancozeb
33	12122-67-7	Zineb
34	759-94-4	EPTC
35	623-80-3	Carbamodithioic acid, S,S-diethyl ester
36	529-34-0	3,4-Dihydro-1(2H)-naphthalenone (α-Tetralone)
37	447-53-0	3,4-Dihydronaphthalene
38	447-53-0	1,2-Dihydronaphthalene
39	119-64-2	1,2,3,4-Tetrahydronaphthalene (Tetralin)
40	825-51-4	Decahydronaphthol-2
41	90-15-3	1-Naphthol
42	135-19-3	2-Naphthol
43	104-90-5	2-Methyl-5-ethylpyridine
44	1696-17-9	N,N-Diethylbenzamide
45	96-45-7	2-Imidazolidinethione (Ethylenethiourea)
46	1563-38-8	2,3-Dihydro-2,2-dimethyl-7-benzofuranol
47	289-16-7	1,2,4-Trithiolane
48	57-14-7	1,1-Dimethylhydrazine
49	540-73-8	1,2-Dimethylhydrazine
50	593-60-2	Bromoethene
51	106-93-4	1,2-dibromoethane
52	30496-13-0	Tetrabromobisphenol A (1,1,3,3-Tetrabromo-2,2-bis(4-phenolyl)propane)
53	108-86-1	Bromobenzene
54	583-53-9	1,2-Dibromobenzene
55	106-37-6	1,4-Dibromobenzene
56	608-21-9	1,2,3-Tribromobenzene
57	626-39-1	1,3,5-Tribromobenzene
58	22311-25-7	1,2,3,4-Tetrabromobenzene
59	634-89-9	1,2,3,5-Tetrabromobenzene
60	608-90-2	Pentabromobenzene
61	87-82-1	Hexabromobenzene
62	608-33-3	2,6-Dibromophenol
63	615-56-5	3,4-Dibromophenol
64	615-58-7	2,4-Dibromophenol
65	626-41-5	3,5-Dibromophenol

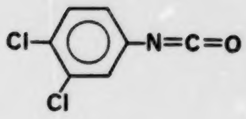
LIST OF DATA SHEETS (continued)

Number	CAS Registry Number	Compound Name
66	28165-52-8	2,5-Dibromophenol
67	28514-45-6	Dibromophenol
68	57383-80-9	2,3-Dibromophenol
69	1163-19-5	Decabromobiphenyl ether
70	32536-52-0	Octabromobiphenyl ether
71	598-94-7	N,N-Dimethylurea
72	689-11-2	sec-Butylurea
73	869-79-4	Di-sec-butylurea
74	4128-34-7	Di-isopropylurea

LIST OF SOURCE CODES

Calc	Molecular weight/oxygen ratio was calculated directly.
CC-Kow	Value of the octanol/water partition coefficient (K_{ow}) was obtained by computer calculation using FRAGMENT calculation procedure (see Section 4.4).
C-OX	Oxidation rate constants were calculated, using functional group reactivity toward alkyl peroxyl radical (RO2) and singlet oxygen (SO).
C-Sw f Kow	The water solubility (S_w) was calculated from the octanol/water partition coefficient (K_{ow}) using the equation of Yalkowsky and Valvani (1980); the calculation of S_w values is discussed in Section 2.
C-vp f bp	Vapor pressure (vp) was calculated from the boiling point (bp) using the method discussed by Grain (1982); the method is discussed in Section 2.
E-A-Carbaryl	Estimated by analogy to Carbaryl; hydrolysis data for Carbaryl from Mabey and Mill (1978).
E-A-Dibromopropane	Estimate by analogy to dibromopropane; hydrolysis data for dibromopropane from Vogel (1983).
E-A-MeBz	Estimate by analogy to methyl benzoate; hydrolysis data for methyl benzoate from Mabey and Mill (1978).
E-A-TDI	Estimated by analogy to toluene diisocyanate; hydrolysis data for toluene diisocyanate from Sopach and Boltromeyuk (1974).
E-KB	Estimate of biotransformation rate constant (k_b) is based on relative rates of transformation reported in literature or on structure-reactivity analogies.
HNES	Hydrolysis is not environmentally significant. Chemical hydrolysis occurs only at extreme pHs or temperatures or with catalysts not available in aquatic environments.
INERT	Oxidation reactions at ambient oxygen levels have half-life greater than 2 years and are therefore considered unimportant fate processes.

M-OX	Oxidation rate constants were modelled using functional group reactivity toward alkyl peroxyl radical (RO2) and singlet oxygen (SO).
NHFG	No hydrolyzable functional groups in molecule.
partial	Partial notation indicates that the computer calculated octanol/water partition coefficient has not accounted for each functional moiety of the molecule. This occurs when a substituent fragment is not represented in the data base or when there are possible hydrogen bonding interactions.
PNER	Photolysis is not environmentally relevant.
RO2	Alkyl peroxyl radical, RO_2.
SO	Singlet oxygen, $^1O_2$
VF-NBD	Volatilization is too fast for biotransformation studies to be conducted. No biotransformation data are therefore available.



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Compound Name: 3,4-dichlorophenylisocyanate

CAS Registry Number: 102-36-6 Molecular Weight(g): 188

Parameters:		Reference
Water Solubility (ppm)	260	C-Sw f Kow
Boiling Point (°C)	161.9/100 torr	Boublik, et al. (1973)
Vapor Pressure (torr)	2.82×10^{-1}	Dean (1979)
Molecular Weight/Oxygen	5.88	Calc
Log (Octanol/Water Partition Coefficient)	3.30 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})	3×10^{-5}	E-A-TDI
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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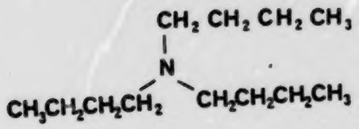

Compound Name: tributylamine

CAS Registry Number: 102-82-9 Molecular Weight(g): 185.4

Parameters:		Reference
Water Solubility (ppm)	31	C-Sw f Kow
Boiling Point (°C)	216-217	Merck (1976)
Vapor Pressure (torr)	0.29	C-vp f bp
Molecular Weight/Oxygen	5.79	Calc
Log (Octanol/Water Partition Coefficient)	4.15	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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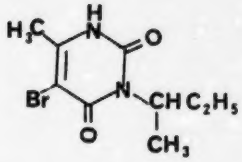

Compound Name: Bromacil

CAS Registry Number: 314-40-9 Molecular Weight(g): 261.11

Parameters:		Reference
Water Solubility (ppm)	815	Spencer (1973)
Melting Point (°C)	157.5-160	Merck (1976)
Boiling Point (°C)	sublimes	Spencer (1973)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	8.16	Calc
Log (Octanol/Water Partition Coefficient)	1.32 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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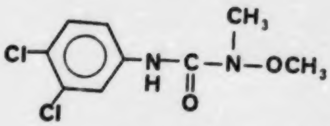
WORK ASSIGNMENT NO. 15



Compound Name: Linuron

CAS Registry Number: 330-55-2 Molecular Weight(g): 249.11

Parameters:		Reference
Water Solubility (ppm)	75	Spencer (1973)
Melting Point (°C)	93-94	Merck (1976)
Boiling Point (°C)		
Vapor Pressure (torr)	1.1 x 10^{-2}/24°C	Spencer (1973)
Molecular Weight/Oxygen	7.78	Calc
Log (Octanol/Water Partition Coefficient)	1.17 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	Aly (1976)
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	Aly (1976)
Neutral Hydrolysis Rate Constant (hr^{-1})	HNES	Aly (1976)
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1 x 10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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$CH_3-S-S-CH_3$

Compound Name: dimethyldisulfide (2,3-dithiabutane)

CAS Registry Number: 624-92-0 Molecular Weight(g): 94.20

Parameters:		Reference
Water Solubility (ppm)	5.2×10^5	C-Sw f Kow
Boiling Point (°C)	112-118	Verschueren (1977)
Vapor Pressure (torr)	28.69	Osborn and Douslin (1966)
Molecular Weight/Oxygen	2.94	Calc
Log (Octanol/Water Partition Coefficient)	-0.04	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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EPA CONTRACT 68-03-2981
WORK ASSIGNMENT NO. 15

$C_2H_5-S-S-C_2H_5$

Compound Name: diethyldisulfide (3,4-dithiahexane)

CAS Registry Number: 110-81-6 Molecular Weight(g): 122.25

Parameters:		Reference
Water Solubility (ppm)	4.6×10^4	C-Sw f Kow
Boiling Point (°C)	154	Weast (1973)
Vapor Pressure (torr)	4.28	Dreisbach (1961)
Molecular Weight/Oxygen	3.82	Calc
Log (Octanol/Water Partition Coefficient)	1.04	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

EPA CONTRACT 68-03-2981
WORK ASSIGNMENT NO. 15

$C_2H_5-S-S-C_3H_7$

Compound Name: ethylpropyldisulfide (3,4-dithiaheptane)

CAS Registry Number: 30453-31-7 Molecular Weight(g): 136.27

Parameters:		Reference
Water Solubility (ppm)	1.3×10^4	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.26	Calc
Log (Octanol/Water Partition Coefficient)	1.58	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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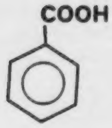
WORK ASSIGNMENT NO. 15



Compound Name: benzoic acid

CAS Registry Number: 68-85-0 Molecular Weight(g): 122.12

Parameters:		Reference
Water Solubility (ppm)	3400	Merck (1976)
Melting Point (°C)	122.4	Merck (1976)
Boiling Point (°C)	249.2	Merck (1976)
Vapor Pressure (torr)	1.26×10^{-3}	Wiedemann (1972)
Molecular Weight/Oxygen	3.82	Calc
Log (Octanol/Water Partition Coefficient)	1.87	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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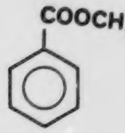

Compound Name: methylbenzoate

CAS Registry Number: 93-58-3 Molecular Weight(g): 136.16

Parameters:		Reference
Water Solubility (ppm)	2600	C-Sw f Kow
Boiling Point (°C)	199.6	Weast (1973)
Vapor Pressure (torr)	0.3944	Dreisbach (1955)
Molecular Weight/Oxygen	4.26	Calc
Log (Octanol/Water Partition Coefficient)	2.24	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	7	Mabey and Mill (1978)
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	1×10^{-3}	Mabey and Mill (1978)
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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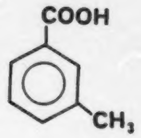

Compound Name: 3-methylbenzoic acid

CAS Registry Number: 99-04-7 Molecular Weight(g): 136.16

Parameters:		Reference
Water Solubility (ppm)	180	C-Sw f Kow
Melting Point (°C)	108.75	Verschueren (1977)
Boiling Point (°C)	263	Verschueren (1977)
Vapor Pressure (torr)	9.6×10^{-4}	C-vp f bp
Molecular Weight/Oxygen	4.26	Calc
Log (Octanol/Water Partition Coefficient)	2.54	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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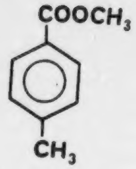

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Compound Name: 4-methylbenzoate

CAS Registry Number: 99-94-3 Molecular Weight(g): 150

Parameters:		Reference
Water Solubility (ppm)	550	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)	4.56×10^{-1}	Weast (1973)
Molecular Weight/Oxygen	4.69	Calc
Log (Octanol/Water Partition Coefficient)	2.90	CC-Kow
Alkaline Hydrolysis Rate Constant $(M^{-1}hr^{-1})$	1×10^{-3}	E-A-MeBz
Acid Hydrolysis Rate Constant $(M^{-1}hr^{-1})$	7	E-A-MeBz
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant $(ml\ cell^{-1}hr^{-1})$	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant $(M^{-1}hr^{-1})$	INERT	M-OX RO2, SO

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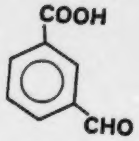

Compound Name: 3-formylbenzoic acid

CAS Registry Number: 619-21-6 Molecular Weight(g): 150.14

Parameters:		Reference
Water Solubility (ppm)	1100	C-Sw f Kow
Melting Point (°C)	175	Weast (1973)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.69	Calc
Log (Octanol/Water Partition Coefficient)	1.23	CC-Kow
Alkaline Hydrolysis Rate Constant (M^{-1}hr^{-1})	NHFG	
Acid Hydrolysis Rate Constant (M^{-1}hr^{-1})	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml cell^{-1}hr^{-1})	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant (M^{-1}hr^{-1})	INERT	M-OX RO2, SO

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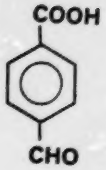

Compound Name: 4-formylbenzoic acid

CAS Registry Number: 619-66-9 Molecular Weight(g): 150.14

Parameters:		Reference
Water Solubility (ppm)	170	C-Sw f Kow
Melting Point (°C)	256	Weast (1973)
Boiling Point (°C)	sublimes	Weast (1973)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.69	Calc
Log (Octanol/Water Partition Coefficient)	1.23	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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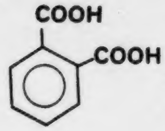

Compound Name: phthalic acid

CAS Registry Number: 88-99-3 Molecular Weight(g): 166.13

Parameters:		Reference
Water Solubility (ppm)	320	C-Sw f Kow
Melting Point (°C)	191 (decomposes)	Hawley (1977)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	5.19	Calc
Log (Octanol/Water Partition Coefficient)	1.62	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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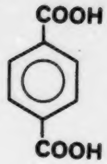

Compound Name: terephthalic acid

CAS Registry Number: 100-21-0

Molecular Weight(g): 166.13

Parameters:		Reference
Water Solubility (ppm)	26	C-Sw f Kow
Boiling Point (°C)	300 (sublimes)	Merck (1976)
Vapor Pressure (torr)	0.15/20°C	Weber et al. (1981)
Molecular Weight/Oxygen	5.19	Calc
Log (Octanol/Water Partition Coefficient)	1.62	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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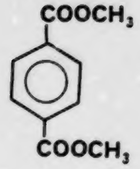

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Compound Name: dimethylterephthalate

CAS Registry Number: 120-61-6 Molecular Weight(g): 194.19

Parameters:		Reference
Water Solubility (ppm)	200	C-Sw f Kow
Melting Point (°C)	140	Verschueren (1977)
Boiling Point (°C)	300 (sublimes)	Verschueren (1977)
Vapor Pressure (torr)	7.0×10^{-5}	C-vp f bp
Molecular Weight/Oxygen	6.07	Calc
Log (Octanol/Water Partition Coefficient)	2.34	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	7	E-A-MeBz
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	1×10^{-3}	E-A-MeBz
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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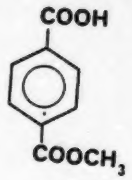

Compound Name: methylterephthalate

CAS Registry Number: 1679-64-7 Molecular Weight(g): 180.19

Parameters:		Reference
Water Solubility (ppm)	6600	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	5.63	Calc
Log (Octanol/Water Partition Coefficient)	1.98	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	7	E-A-MeBz
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	1×10^{-3}	E-A-MeBz
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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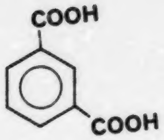

Compound Name: isophthalic acid

CAS Registry Number: 121-91-5 Molecular Weight(g): 166.13

Parameters:		**Reference**
Water Solubility (ppm)	130	Verschueren (1977)
Melting Point (°C)	345-348	Merck (1976)
Boiling Point (°C)	sublimes	Merck (1976)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	5.19	Calc
Log (Octanol/Water Partition Coefficient)	1.62	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX, RO2, SO

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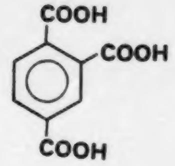

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Compound Name: trimellitic acid (1,2,4-benzenetricarboxylic acid)

CAS Registry Number: 528-44-9 Molecular Weight(g): 210.14

Parameters:		Reference
Water Solubility (ppm)	400	C-Sw f Kow
Melting Point (°C)	218-220	Merck (1976)
Melting Point (°C)	238 (decomposes)	Weast (1973)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	6.57	Calc
Log (Octanol/Water Partition Coefficient)	1.37	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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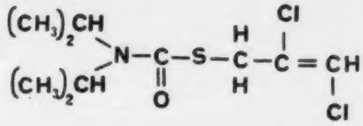

Compound Name: Diallate

CAS Registry Number: 2303-16-4 Molecular Weight(g): 273.5

Parameters:		Reference
Water Solubility (ppm)	14	Spencer (1973)
Boiling Point (°C)	150/9 torr	Merck (1976)
Vapor Pressure (torr)	6.8×10^{-3}	C-vp f bp
Molecular Weight/Oxygen	8.55	Calc
Log (Octanol/Water Partition Coefficient)	0.73 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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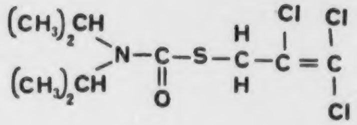

Compound Name: Triallate

CAS Registry Number: 2303-17-5 Molecular Weight(g): 305

Parameters:		Reference
Water Solubility (ppm)	4	Spencer (1973)
Melting Point (°C)	29-30	Spencer (1973)
Boiling Point (°C)	148-149/9 torr	Spencer (1973)
Vapor Pressure (torr)	2.07×10^{-4}	Grover et al. (1978)
Molecular Weight/Oxygen	9.53	Calc
Log (Octanol/Water Partition Coefficient)	1.33 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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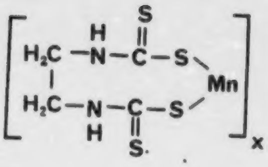

Compound Name: Maneb

CAS Registry Number: 12427-38-2 Molecular Weight(g): 265.29

Parameters:		Reference
Water Solubility (ppm)		
Boiling Point (°C)	decomposes before melting	Spencer (1973)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	8.29	Calc
Log (Octanol/Water Partition Coefficient)		
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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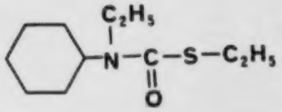

Compound Name: Cycloate

CAS Registry Number: 1134-23-2 Molecular Weight(g): 215.4

Parameters:		Reference
Water Solubility (ppm)	75/20°C	Spencer (1973)
Boiling Point (°C)	146/10 torr	Spencer (1973)
Vapor Pressure (torr)	6.2×10^{-3}	Spencer (1973)
Molecular Weight/Oxygen	6.72	Calc
Log (Octanol/Water Partition Coefficient)	1.85	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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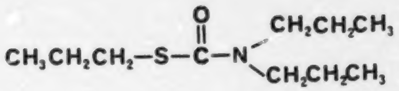

$CH_3CH_2CH_2-S-\overset{O}{\overset{\|}{C}}-N\begin{matrix}CH_2CH_2CH_3\\ CH_2CH_2CH_3\end{matrix}$

Compound Name: Vernolate

CAS Registry Number: 1929-77-7 Molecular Weight(g): 203.1

Parameters:		Reference
Water Solubility (ppm)	90/20°C	Spencer (1973)
Boiling Point (°C)	140/20 torr	Spencer (1973)
Vapor Pressure (torr)	1.04×10^{-2}	Spencer (1973)
Molecular Weight/Oxygen	6.16	Calc
Log (Octanol/Water Partition Coefficient)	1.84	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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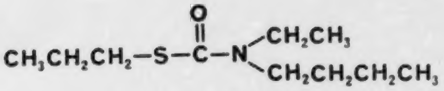

$CH_3CH_2CH_2{-}S{-}\overset{\overset{O}{\|}}{C}{-}N\begin{matrix}\diagup CH_2CH_3\\ \diagdown CH_2CH_2CH_2CH_3\end{matrix}$

Compound Name: Pebulate

CAS Registry Number: 1114-71-2 Molecular Weight(g): 203.36

Parameters:		Reference
Water Solubility (ppm)	92/21°C	Spencer (1973)
Boiling Point (°C)	142/20 torr	Merck (1976)
Vapor Pressure (torr)	3.5×10^{-2} 3.3×10^{-2}	Ouellette and King (1977) C-vp f bp
Molecular Weight/Oxygen	6.36	Calc
Log (Octanol/Water Partition Coefficient)	1.84	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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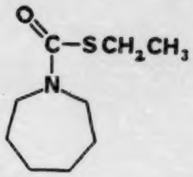

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Compound Name: Molinate

CAS Registry Number: 2212-67-1 Molecular Weight(g): 187.1

Parameters:		Reference
Water Solubility (ppm)	912/21°C	Spencer (1973)
Boiling Point (°C)	137/10 torr	Spencer (1973)
Vapor Pressure (torr)	5.6×10^{-3} 1.9×10^{-2}	Ouellette and King (1977) C-vp f bp
Molecular Weight/Oxygen	5.84	Calc
Log (Octanol/Water Partition Coefficient)	0.90	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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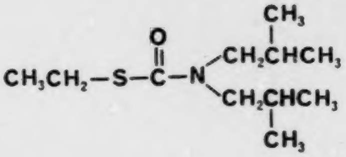
WORK ASSIGNMENT NO. 15



Compound Name: Butylate

CAS Registry Number: 2008-41-5 Molecular Weight(g): 217.4

Parameters:		Reference
Water Solubility (ppm)	36/20°C	Spencer (1973)
Boiling Point (°C)	138/21.5 torr	Spencer (1973)
Vapor Pressure (torr)	1.3×10^{-2}	Spencer (1973)
Molecular Weight/Oxygen	6.79	Calc
Log (Octanol/Water Partition Coefficient)	2.12	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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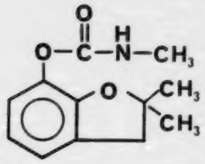

Compound Name: Carbofuran

CAS Registry Number: 1563-66-2 Molecular Weight(g): 221.3

Parameters:		Reference
Water Solubility (ppm)	700	Spencer (1973)
Melting Point (°C)	150-153	Merck (1976)
Boiling Point (°C)		
Vapor Pressure (torr)	$<1.4 \times 10^{-5}$	Jaber et al. (1983)
Molecular Weight/Oxygen	6.91	Calc
Log (Octanol/Water Partition Coefficient)	2.55	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	1638	E-A-Carbaryl
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	5.04×10^{-4}	E-A-Carbaryl
Neutral Hydrolysis Rate Constant (hr^{-1})	2.5×10^{-3}	E-A-Carbaryl
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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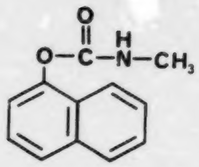

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Compound Name: Carbaryl

CAS Registry Number: 63-25-2 Molecular Weight(g): 201.2

Parameters:		Reference
Water Solubility (ppm)	40/30°C	Spencer (1973)
Melting Point (°C)	145	Merck (1976)
Boiling Point (°C)		
Vapor Pressure (torr)	$<6 \times 10^{-6}$	Jaber et al. (1983)
Molecular Weight/Oxygen	6.28	Calc
Log (Octanol/Water Partition Coefficient)	2.50	CC-Kow
Alkaline Hydrolysis Rate Constant $(M^{-1}hr^{-1})$	1638	Mabey and Mill (1978)
Acid Hydrolysis Rate Constant $(M^{-1}hr^{-1})$	5×10^{-4}	Mabey and Mill (1978)
Neutral Hydrolysis Rate Constant (hr^{-1})	2.5×10^{-3}	Mabey and Mill (1978)
Microbial Degradation Rate Constant $(ml\ cell^{-1}hr^{-1})$	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant $(M^{-1}hr^{-1})$	INERT	M-OX RO2, SO

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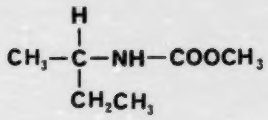

$CH_3-\overset{\displaystyle H}{\underset{\displaystyle CH_2CH_3}{C}}-NH-COOCH_3$

Compound Name: sec-butylcarbamic acid, methyl ester

CAS Registry Number: 39076-02-3 Molecular Weight(g): 131

Parameters:		Reference
Water Solubility (ppm)	2.1×10^4	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.09	Calc
Log (Octanol/Water Partition Coefficient)	1.39	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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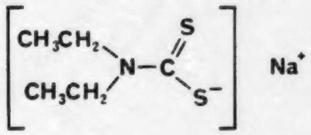

Compound Name: Dithiocarbamate

CAS Registry Number: 148-18-5 Molecular Weight(g): 171.27

Parameters:		Reference
Water Solubility (ppm)	1.2×10^5	C-Sw f Kow
Melting Point (°C)	94-96	Merck (1976)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	5.35	Calc
Log (Octanol/Water Partition Coefficient)	0.04 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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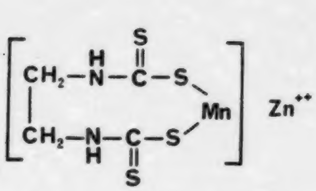

Compound Name: Mancozeb

CAS Registry Number: 8018-01-7 Molecular Weight(g): 540

Parameters:		Reference
Water Solubility (ppm)		
Boiling Point (°C)	decomposes before melting	Spencer (1973)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	16.86	Calc
Log (Octanol/Water Partition Coefficient)		
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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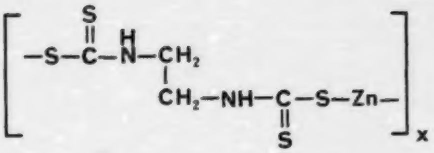

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Compound Name: Zineb

CAS Registry Number: 12122-67-7 Molecular Weight(g): $(275.7)_x$

Parameters:		Reference
Water Solubility (ppm)	10	Spencer (1973)
Boiling Point (°C)	decomposes before melting	Spencer (1973)
Vapor Pressure (torr)	negligible	Spencer (1973)
Molecular Weight/Oxygen	8.62	Calc
Log (Octanol/Water Partition Coefficient)		
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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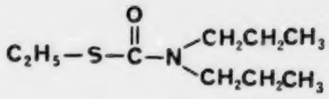

Compound Name: EPTC

CAS Registry Number: 759-94-4 Molecular Weight(g): 189.3

Parameters:		Reference
Water Solubility (ppm)	375/20°C	Spencer (1973)
Boiling Point (°C)	137-138/30 torr	Spencer (1973)
Vapor Pressure (torr)	3.4×10^{-2}	Spencer (1973)
Molecular Weight/Oxygen	5.92	Calc
Log (Octanol/Water Partition Coefficient)	1.30	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX R02, SO

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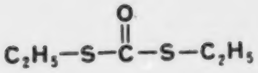

$C_2H_5-S-\overset{\overset{O}{\|}}{C}-S-C_2H_5$

Compound Name: carbamodithioic acid, S,S-diethyl ester

CAS Registry Number: 623-80-3 Molecular Weight(g): 150

Parameters:		Reference
Water Solubility (ppm)	1.7×10^6	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.69	Calc
Log (Octanol/Water Partition Coefficient)	-0.32	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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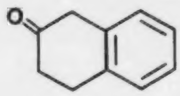

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Compound Name: 3,4-dihydro-1(2H)-naphthalenone (α-tetralone)

CAS Registry Number: 529-34-0 Molecular Weight(g): 146.19

Parameters:		Reference
Water Solubility (ppm)	1.6 X 10^{4}	C-Sw f Kow
Melting Point (°C)	5.3-6	Aldrich (1982)
Boiling Point (°C)	113-116/6 torr	Aldrich (1982)
Vapor Pressure (torr)	3.0 x 10^{-2}	C-vp f bp
Molecular Weight/Oxygen	4.57	Calc
Log (Octanol/Water Partition Coefficient)	1.53	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1 x 10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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37
same as 38

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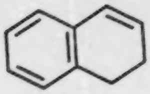

Compound Name: 3,4-dihydronaphthalene

CAS Registry Number: 447-53-0 Molecular Weight(g): 130.19

Parameters:		Reference
Water Solubility (ppm)	98	C-Sw f Kow
Boiling Point (°C)	206-207	Weast (1973)
Vapor Pressure (torr)	0.51	C-vp f bp
Molecular Weight/Oxygen	4.07	Calc
Log (Octanol/Water Partition Coefficient)	3.54	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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same as 37

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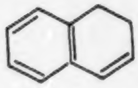

Compound Name: 1,2-dihydronaphthalene

CAS Registry Number: 447-53-0 Molecular Weight(g): 130.19

Parameters:		Reference
Water Solubility (ppm)	98	C-Sw f Kow
Boiling Point (°C)	206-207	Weast (1973)
Vapor Pressure (torr)	0.51	C-vp f bp
Molecular Weight/Oxygen	4.07	Calc
Log (Octanol/Water Partition Coefficient)	3.54	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	4×10^{5}	M-OX RO2

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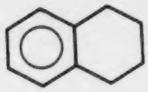

Compound Name: 1,2,3,4-tetrahydronaphthalene (Tetralin)

CAS Registry Number: 119-64-2 Molecular Weight(g): 132.2

Parameters:		Reference
Water Solubility (ppm)	35	C-Sw f Kow
Boiling Point (°C)	207.6	Dreisbach (1955)
Vapor Pressure (torr)	0.3869	Dreisbach (1955)
Molecular Weight/Oxygen	4.13	Calc
Log (Octanol/Water Partition Coefficient)	3.96	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2

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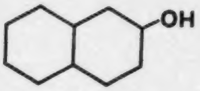

Compound Name: decahydronaphthol-2

CAS Registry Number: 825-51-4 Molecular Weight(g): 154.25

Parameters:		Reference
Water Solubility (ppm)	300	C-Sw f Kow
Boiling Point (°C)	109/14 torr	Aldrich (1982)
Vapor Pressure (torr)	1.18×10^{-2}	Jaber et al. (1983)
Molecular Weight/Oxygen	4.82	Calc
Log (Octanol/Water Partition Coefficient)	3.15	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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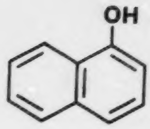

Compound Name: 1-naphthol

CAS Registry Number: 90-15-3 Molecular Weight(g): 144.16

Parameters:		Reference
Water Solubility (ppm)	210	C-Sw f Kow
Melting Point (°C)	96	Merck (1976)
Boiling Point (°C)	288	Merck (1976)
Vapor Pressure (torr)	1.07×10^{-4}	C-vp f bp
Molecular Weight/Oxygen	4.51	Calc
Log (Octanol/Water Partition Coefficient)	2.62	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	7×10^{8}	M-OX RO2

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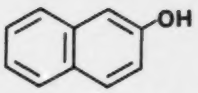

Compound Name: 2-naphthol

CAS Registry Number: 135-19-3 Molecular Weight(g): 144.16

Parameters:		Reference
Water Solubility (ppm)	740	Verschueren (1977)
Melting Point (°C)	122	Verschueren (1977)
Boiling Point (°C)	285-286	Merck (1976)
Vapor Pressure (torr)	2.24×10^{-4}	Karyakin et al. (1968)
Molecular Weight/Oxygen	4.51	Calc
Log (Octanol/Water Partition Coefficient)	2.62	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-7}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{8}	M-OX RO2

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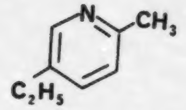

Compound Name: 2-methyl-5-ethylpyridine

CAS Registry Number: 104-90-5 Molecular Weight(g): 121.18

Parameters:		Reference
Water Solubility (ppm)	1100	C-Sw f Kow
Boiling Point (°C)	179.3	Boublik et al. (1973)
Vapor Pressure (torr)	1.13	Van De Rostyne and Prausnitz (1980)
Molecular Weight/Oxygen	3.78	Calc
Log (Octanol/Water Partition Coefficient)	2.53	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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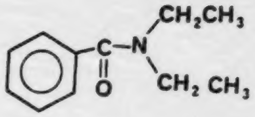

Compound Name: N,N-diethylbenzamide

CAS Registry Number: 1696-17-9 Molecular Weight(g): 137

Parameters:		Reference
Water Solubility (ppm)	7100	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.28	Calc
Log (Octanol/Water Partition Coefficient)	1.84	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant ($ml\ cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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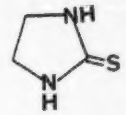

Compound Name: 2-imidazolidinethione (ethylenethiourea)

CAS Registry Number: 96-45-7 Molecular Weight(g): 102.16

Parameters:		Reference
Water Solubility (ppm)	1.1×10^{5}	C-Sw f Kow
Melting Point (°C)	203-204	Merck (1976)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	3.19	Calc
Log (Octanol/Water Partition Coefficient)	-1.03 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	4×10^{10}	M-OX SO

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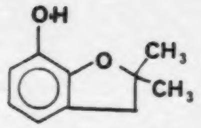

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Compound Name: 2,3-dihydro-2,2-dimethyl-7-benzofuranol

CAS Registry Number: 1563-38-8 Molecular Weight(g): 220

Parameters:		Reference
Water Solubility (ppm)	700	Merck (1976)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	6.87	Calc
Log (Octanol/Water Partition Coefficient)	2.60	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

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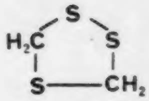

Compound Name: 1,2,4-trithiolane

CAS Registry Number: 289-16-7 Molecular Weight(g): 124

Parameters:		Reference
Water Solubility (ppm)	1.7×10^6	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	3.87	Calc
Log (Octanol/Water Partition Coefficient)	-0.40	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	3×10^{10}	M-OX SO

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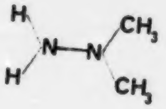

Compound Name: 1,1-dimethylhydrazine

CAS Registry Number: 57-14-7 Molecular Weight(g): 60.10

Parameters:		Reference
Water Solubility (ppm)	1.2×10^{8}	C-Sw f Kow
Boiling Point (°C)	63.9	Merck (1976)
	158	C-vp f bp
Vapor Pressure (torr)	157	Verschueren (1977)
Molecular Weight/Oxygen	1.88	Calc
Log (Octanol/Water Partition Coefficient)	-2.42	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	labile[a]	M-OX RO2

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(a) Reacts with oxygen directly. Half-life estimated to be less than 10 days.

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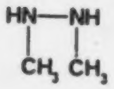

$$\begin{array}{cc} HN & \!\!-\!\!\; NH \\ | & | \\ CH_3 & CH_3 \end{array}$$

Compound Name: 1,2-dimethylhydrazine

CAS Registry Number: 540-73-8 Molecular Weight(g): 60.10

Parameters:		Reference
Water Solubility (ppm)	2.9×10^8	C-Sw f Kow
Boiling Point (°C)	81/753 torr	Merck (1976)
Vapor Pressure (torr)	75 69.9	C-vp f bp Bouhlik, et al. (1973)
Molecular Weight/Oxygen	1.88	Calc
Log (Octanol/Water Partition Coefficient)	-2.76	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	labile[a]	M-OX

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(a) Reacts with oxygen directly. Half-life estimated to be less than 10 days.

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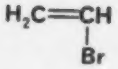

$H_2C{=}CH(Br)$

Compound Name: bromoethene

CAS Registry Number: 593-60-2 Molecular Weight(g): 106.96

Parameters:		Reference
Water Solubility (ppm)	1.7×10^4	C-Sw f Kow
Boiling Point (°C)	15.80	Dreisbach (1959)
Vapor Pressure (torr)	1033	Dreisbach (1959)
Molecular Weight/Oxygen	3.34	Calc
Log (Octanol/Water Partition Coefficient)	1.38	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Neutral Hydrolysis Rate Constant (hr^{-1})	HNES	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	--	VF - NBD
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	C-OX RO2, SO

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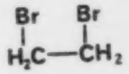

BrH_2C-CH_2Br

Compound Name: 1,2-dibromoethane

CAS Registry Number: 106-93-4

Molecular Weight(g): 187.88

Parameters:		Reference
Water Solubility (ppm)	4300/30°C	Spencer (1973)
Boiling Point (°C)	131-132	Merck (1976)
Vapor Pressure (torr)	11.70	Dreisbach (1959)
Molecular Weight/Oxygen	5.88	Calc
Log (Octanol/Water Partition Coefficient)	1.76	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Neutral Hydrolysis Rate Constant (hr^{-1})	3.7×10^{-5}	E-A-Dibromopropane
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	C-OX RO2, SO

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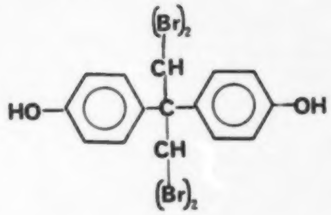

Compound Name: Tetrabromobisphenol A (1,1,3,3-tetrabromo-2,2-bis(4-phenolyl)propane)

CAS Registry Number: 30496-13-0 Molecular Weight(g): 543.8

Parameters:		Reference
Water Solubility (ppm)		
Melting Point (°C)	180-184	Hawley (1977)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	17.0	Calc
Log (Octanol/Water Partition Coefficient)		
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)		
Neutral Hydrolysis Rate Constant (hr^{-1})		
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	2×10^{7}	M-OX RO2

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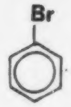

Compound Name: bromobenzene

CAS Registry Number: 108-86-1 Molecular Weight(g): 157.02

Parameters:		Reference
Water Solubility (ppm)	450	C-Sw f Kow
Boiling Point (°C)	156.2	Dreisbach (1955)
Vapor Pressure (torr)	4.18	Dreisbach (1955)
Molecular Weight/Oxygen	4.91	Calc
Log (Octanol/Water Partition Coefficient)	3.00	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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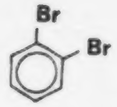

Compound Name: 1,2-dibromobenzene

CAS Registry Number: 583-53-9 Molecular Weight(g): 235.92

Parameters:		Reference
Water Solubility (ppm)	80	C-Sw f Kow
Boiling Point (°C)	224	Aldrich (1982)
Vapor Pressure (torr)	0.193	Dreisbach (1955)
Molecular Weight/Oxygen	7.37	Calc
Log (Octanol/Water Partition Coefficient)	3.86	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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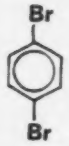

Compound Name: 1,4-dibromobenzene

CAS Registry Number: 106-37-6 Molecular Weight(g): 235.92

Parameters:		Reference
Water Solubility (ppm)	19	C-Sw f Kow
Melting Point (°C)	87-89	Aldrich (1982)
Boiling Point (°C)	220.4	Merck (1976)
Vapor Pressure (torr)	0.025	Jordan (1954)
Molecular Weight/Oxygen	7.37	Calc
Log (Octanol/Water Partition Coefficient)	3.86	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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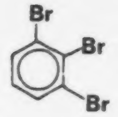

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Compound Name: 1,2,3-tribromobenzene

CAS Registry Number: 608-21-9 Molecular Weight(g): 314.82

Parameters:		Reference
Water Solubility (ppm)	12	C-Sw f Kow
Melting Point (°C)	87.8	Weast (1973)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	9.84	Calc
Log (Octanol/Water Partition Coefficient)	4.73	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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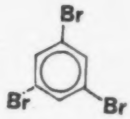
EPA CONTRACT 68-03-2981
WORK ASSIGNMENT NO. 15



Compound Name: 1,3,5-tribromobenzene

CAS Registry Number: 626-39-1 Molecular Weight(g): 314.82

Parameters:		Reference
Water Solubility (ppm)	1.3	C-Sw f Kow
Melting Point (°C)	121-124	Aldrich (1982)
Boiling Point (°C)	271/765 torr	Weast (1973)
Vapor Pressure (torr)	6.4×10^{-4}	C-vp f bp
Molecular Weight/Oxygen	9.84	Calc
Log (Octanol/Water Partition Coefficient)	4.73	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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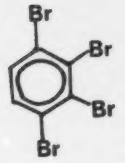

Compound Name: 1,2,3,4-tetrabromobenzene

CAS Registry Number: 22311-25-7 Molecular Weight(g): 393.72

Parameters:		Reference
Water Solubility (ppm)	1.8	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	12.30	Calc
Log (Octanol/Water Partition Coefficient)	5.59	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

- These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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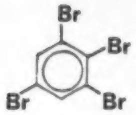

Compound Name: 1,2,3,5-tetrabromobenzene

CAS Registry Number: 634-89-9 Molecular Weight(g): 393.72

Parameters:		Reference
Water Solubility (ppm)	1.8	C-Sw f Kow
Melting Point (°C)	99-100	Weast (1973)
Boiling Point (°C)	329	Weast (1973)
Vapor Pressure (torr)	1.3×10^{-6}	C-vp f bp
Molecular Weight/Oxygen	12.30	Calc
Log (Octanol/Water Partition Coefficient)	5.59	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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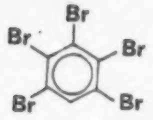

Compound Name: pentabromobenzene

CAS Registry Number: 608-90-2 Molecular Weight(g): 472.6

Parameters:		Reference
Water Solubility (ppm)	0.25	C-Sw f Kow
Melting Point (°C)	160-161	Weast (1973)
Boiling Point (°C)	sublimes	Weast (1973)
Vapor Pressure (torr)		
Molecular Weight/Oxygen	14.77	Calc
Log (Octanol/Water Partition Coefficient)	6.46	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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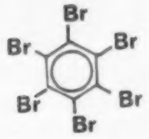

Compound Name: hexabromobenzene

CAS Registry Number: 87-82-1 Molecular Weight(g): 551.52

Parameters:		Reference
Water Solubility (ppm)	9×10^{-6}	C-Sw f Kow
Melting Point (°C)	327	Weast (1973)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	17.2	Calc
Log (Octanol/Water Partition Coefficient)	7.32	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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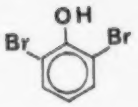

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Compound Name: 2,6-dibromophenol

CAS Registry Number: 608-33-3 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	210	C-Sw f Kow
Melting Point (°C)	56-7	Weast (1973)
Boiling Point (°C)	162/21 torr (sublimes)	Weast (1973)
Vapor Pressure (torr)	2.5×10^{-3}	C-vp f bp
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	1×10^{-10}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

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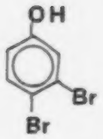

Compound Name: 3,4-dibromophenol

CAS Registry Number: 615-56-5 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	440	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

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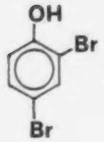

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Compound Name: 2,4-dibromophenol

CAS Registry Number: 615-58-7 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	310	C-Sw f Kow
Melting Point (°C)	40	Weast (1973)
Boiling Point (°C)	238-9	Weast (1973)
Vapor Pressure (torr)	1.9×10^{-3}	C-vp f bp
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

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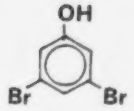
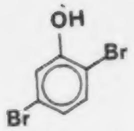


Compound Name: 3,5-dibromophenol

CAS Registry Number: 626-41-5 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	440	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.



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WORK ASSIGNMENT NO. 15

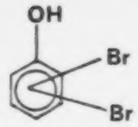
Compound Name: 2,5-dibromophenol

CAS Registry Number: 28165-52-8 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	440	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

EPA CONTRACT 68-03-2981
WORK ASSIGNMENT NO. 15



Compound Name: dibromophenol

CAS Registry Number: 28514-45-6 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	440	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2, SO

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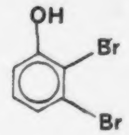
WORK ASSIGNMENT NO. 15



Compound Name: 2,3-dibromophenol

CAS Registry Number: 57383-80-9 Molecular Weight(g): 251.9

Parameters:		Reference
Water Solubility (ppm)	440	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	7.87	Calc
Log (Octanol/Water Partition Coefficient)	3.20 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	1×10^{7}	M-OX RO2

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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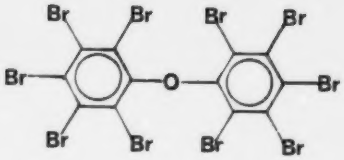
WORK ASSIGNMENT NO. 15



Compound Name: decabromobiphenyl ether

CAS Registry Number: 1163-19-5 Molecular Weight(g): 959.22

Parameters:		Reference
Water Solubility (ppm)	1.3×10^{13}	C-Sw f Kow
Melting Point (°C)	294 - 296	Fluka (1982)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	30.00	Calc
Log (Octanol/Water Partition Coefficient)	12.87 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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Compound Name: octabromobiphenyl ether

CAS Registry Number: 32536-52-0 Molecular Weight(g): 442

Parameters:		Reference
Water Solubility (ppm)		
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	13.81	Calc
Log (Octanol/Water Partition Coefficient)		
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	NHFG	
Neutral Hydrolysis Rate Constant (hr^{-1})	NHFG	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-12}	E-KB
Photolysis Rate Constant (hr^{-1})		
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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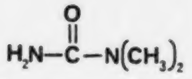
WORK ASSIGNMENT NO. 15



$H_2N-\overset{\overset{\displaystyle O}{\|}}{C}-N(CH_3)_2$

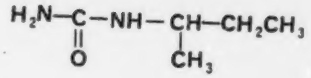
Compound Name: N,N-dimethylurea

CAS Registry Number: 598-94-7 Molecular Weight(g): 88.11

Parameters:		Reference
Water Solubility (ppm)	7100	C-Sw f Kow
Melting Point (°C)	106	Hawley (1977)
Boiling Point (°C)	270	Hawley (1977)
Vapor Pressure (torr)	5.9×10^{-4}	C-vp f bp
Molecular Weight/Oxygen	2.75	Calc
Log (Octanol/Water Partition Coefficient)	1.66 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Neutral Hydrolysis Rate Constant (hr^{-1})	HNES	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

EPA CONTRACT 68-03-2981
WORK ASSIGNMENT NO. 15


$H_2N-C(=O)-NH-CH(CH_3)-CH_2CH_3$

Compound Name: sec-butylurea

CAS Registry Number: 689-11-2 Molecular Weight(g): 116.16

Parameters:		Reference
Water Solubility (ppm)	4.4×10^5	C-Sw f Kow
Melting Point (°C)	169-170	Weast (1973)
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	3.63	Calc
Log (Octanol/Water Partition Coefficient)	0.11	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Neutral Hydrolysis Rate Constant (hr^{-1})	HNES	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

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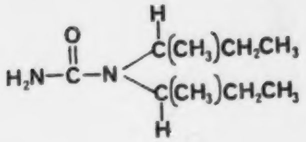

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Compound Name: di-sec-butylurea

CAS Registry Number: 869-79-4 Molecular Weight(g): 172

Parameters:		Reference
Water Solubility (ppm)	13	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	5.38	Calc
Log (Octanol/Water Partition Coefficient)	4.46 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Neutral Hydrolysis Rate Constant (hr^{-1})	HNES	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

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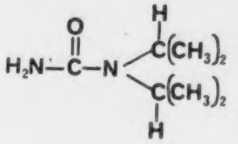
WORK ASSIGNMENT NO. 15



Compound Name: di-isopropylurea

CAS Registry Number: 4128-34-7 Molecular Weight(g): 142

Parameters:		Reference
Water Solubility (ppm)	160	C-Sw f Kow
Boiling Point (°C)		
Vapor Pressure (torr)		
Molecular Weight/Oxygen	4.43	Calc
Log (Octanol/Water Partition Coefficient)	3.38 (partial)	CC-Kow
Alkaline Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Acid Hydrolysis Rate Constant ($M^{-1}hr^{-1}$)	HNES	
Neutral Hydrolysis Rate Constant (hr^{-1})	HNES	
Microbial Degradation Rate Constant (ml $cell^{-1}hr^{-1}$)	3×10^{-9}	E-KB
Photolysis Rate Constant (hr^{-1})	PNER	
Oxidation Rate Constant ($M^{-1}hr^{-1}$)	INERT	M-OX RO2, SO

These data were estimated for use in a preliminary assessment to be conducted by the EPA, and should not be used in more detailed assessments.

REFERENCES

Aldrich Chemical Company. 1982-1983. Aldrich Catalog/Handbook of Fine Chemicals. Milwaukee, Wisconsin.

Aly, O. A. 1976. Water Res. 10, No. 12, 1047-1050.

Boublik, T., V. Fried, and E. Hala. 1973. The Vapour Pressures of Pure Substances. Elsevier Scientific Publishing Co., Amsterdam.

Dean, J. A., Ed. 1979. Lange's Handbook of Chemistry, Twelfth Edition. McGraw-Hill Book Co., New York.

Dreisbach, R. R. 1955. Physical Properties of Chemical Compounds. Advances in Chemistry Series No. 15. American Chemical Society, Washington, DC.

Dreisbach, R. R. 1959. Physical Properties of Chemical Compounds-II. Advances in Chemistry Series No. 22. American Chemical Society, Washington, DC.

Dreisbach, R. R. 1961. Physical Properties of Chemical Compounds-III. Advances in Chemistry Series No. 29. American Chemical Society, Washington, DC.

Fluka Chemical Corporation. 1983/1983 Catalog. Hauppauge, NY.

Grain, C. 1982. Vapor Pressure. In: Handbook of Chemical Property Estimation Methods. W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, Eds. McGraw-Hill Book Company, New York.

Grover, R., W. F. Spencer, W. J. Farmer, and T. D. Shoup. 1978. Weed Sci. 26, No. 5, 505-508.

Hawley, G. G. 1977. The Condensed Chemical Dictionary. Ninth Edition. Van Nostrand Reinhold Co., New York.

Jaber, H. M., K. C. Irwin, and E. C. Gunderson. 1983. Data Acquisition for Environmental Transport and Fate Screening for Compounds of Interest to the Office of Solid Waste. Part II. Vapor Pressure Measurements. Final Report for U. S. EPA, Washington, DC. Work Assignment No. 15 in partial fulfillment of EPA Contract No. 68-03-2981.

Jordan, T. E. 1954. Vapor Pressure of Organic Compounds. Interscience Publishers, Inc., New York.

Karyakin, N. V., I. B. Rabinovich, and L. G. Pakhomov. 1968. Zh. Fiz. Khim. 42, No. 7, 1814-1816.

Mabey, W. R., and T. Mill. 1978. J. Phys. Chem. Ref. Data. 7, No. 2, 383-415.

The Merck Index. 1976. 9th Edition. Merck and Co., Rahway, New Jersey.

Ouellette, R. P., and J. A. King. 1977. Chemical Week Pesticide Register. McGraw-Hill, Co., New York. 345 pp.

Osborn, A. G., and D. R. Douslin. 1966. J. Chem. Eng. Data. 11, No. 4, 502-509.

Sopach, E. D., and L. P. Boltromeyuk. 1974. Gigiena i sanitariya. 7, 10-13.

Spencer, E. Y. 1973. Guide to the Chemicals Used in Crop Protection. Agriculture Canada. Publication 1093, Sixth Edition. Ottawa, Ontario, Canada.

Van De Rostyne, C., and J. M. Prausnitz. 1980. J. Chem. Eng. Data. 25, No. 1, 1-3.

Verschueren, K. 1977. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold Co., New York.

Vogel, T. 1983. Unpublished work. Stanford University, Stanford, CA.

Weast, R. C. Ed. 1973. Handbook of Chemistry and Physics. 54th Edition. CRC Press, Cleveland, OH.

Weber, R. C., P. A. Parker, and M. Bowser. 1981. Vapor Pressure Distribution of Selected Organic Chemicals. EPA Report No. 600/2-81-021.

Wiedemann, H. G. 1972. Thermochim. Acta. 3, No. 5, 355-366.

Yalkowsky, S. H., and S. C. Valvani. 1980. J. Pharm. Sci. 69, No. 8, 912-922.

SECTION 4

CALCULATION OF PARTITION COEFFICIENTS OF ORGANIC CHEMICALS IN AQUATIC ENVIRONMENTS

This section was taken in whole from W. R. Mabey, J. H. Smith, R. T. Podoll, et al., "Aquatic Fate Process Data for Organic Priority Pollutants," EPA Report No. 440/4-81-014, December 1982.

Section 4

CALCULATION OF PARTITION COEFFICIENT OF ORGANIC CHEMICALS IN AQUATIC ENVIRONMENTS *

4.1 BACKGROUND

The partitioning of a chemical between water and sediment and between water and biota will affect the concentration of the chemical in water and the rate of loss of the chemical from aquatic systems. Solubility data, on the other hand, are required for calculation of Henry's constants, which are needed to calculate volatilization rates of chemicals in aquatic systems.

This section discusses the relationships between water solubility, the partition coefficients for a chemical between sediment and biota, and the partition coefficient for a chemical between octanol and water. Moreover, the theoretical basis for such relationships is explained, and some of the published correlations for these data are discussed. This section also briefly discusses the calculation of the octanol-water partition coefficient data used to calculate many of the other partitioning constants.

As discussed in Section 2, the partitioning of a chemical is given by the equation

$$K_p = C_p/C_w \qquad (4.1)$$

where C_p and C_w are the concentrations on a particulate material (sediment or biota) and in water, respectively, and K_p is the partitioning constant (or coefficient) whose units are determined by those of C_p and C_w (see section 2). In practice, C_p is usually defined as the amount of chemical per dry weight of sediment (or organisms) to correct for the variability of the particulate water content. The partition coefficient between

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*This section was taken in whole from W. R. Mabey, J. H. Smith, R. T. Podoll, et al., "Aquatic Fate Process Data for Organic Priority Pollutants," EPA Report No. 440/4-81-014, December 1982.

microorganism and water, K_B, given for individual organic chemicals in Section 3, is in units of micrograms of chemical per gram of microorganism divided by grams of chemical per liter of water. Because the amount of organic chemical sorbed to sediments has been found to depend on the amount of organic carbon in the sediment, it is useful to normalize a measured sediment partition coefficient (K_p) for organic carbon content:

$$K_{oc} = K_p/f_{oc} \qquad (4.2)$$

where f_{oc} is the fraction of organic carbon and K_{oc} is the normalized (for organic carbon content) partition coefficient. Karickhoff et al. (1979) have also shown that, because f_{oc} varies with sediment particle size, the distribution of sediment particle size will markedly affect measured K_{oc} values.

The octanol-water partion coefficient K_{ow} has commonly been used as a measure of the hydrophobicity of a chemical in medical and toxicological applications as well as in environmental chemistry (Hansch and Leo, 1979; Kenaga and Goring, 1978). A large number of K_{ow} values is therefore available as a result of the number of uses of such data. Most significantly, K_{ow} values can be calculated from molecular structure (see Section 4.4). The K_{ow} data in Section 3 are given to allow calculations of other properties (partitioning coefficients for biota as well as toxicological data) for use in environmental assessments of the organic priority pollutants.

4.2 CALCULATION METHODS

Several correlation equations have been proposed to calculate the water solubility (S_w), K_{oc}, and K_B from K_{ow} values and to calculate K_{oc} values from water solubility. The more widely used of these equations are discussed and analyzed in Section 4.3. Although we recognize that better equations are evolving as more experimental data are obtained, the following equations are recommended for use in environmental fate assessments.

4.2.1 Correlation Equations

In the following equations, all partition coefficients (K_{oc}, K_{ow} and K_B) are unitless, and water solubility (S_w) is in units of parts per million (ppm).* As discussed in Section 4.2.2, however, the solubility units of molarity (moles per liter) or mole fraction are preferred.

K_{oc} and K_{ow} are correlated by the following equation (Karickhoff, 1979):

$$\log K_{oc} = 1.00 \log K_{ow} - 0.21 \qquad (4.3)$$

Correlation of S_w and K_{ow} was reported by Yalkowsky and Valvani (1980). For organic pollutants that are liquid in their pure state at 25°C:

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW \qquad (4.4)$$

where MW is the molecular weight of the pollutant (g $mole^{-1}$). For organic pollutants that are solid in their pure state at 25°C:

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW - \left(\frac{\Delta S_F}{1360}\right)(mp-25) \qquad (4.5)$$

where mp is the melting point of the pollutant (°C) and ΔS_f is the entropy of fusion of the pollutant (cal mol^{-1} deg^{-1}). If ΔS_f is not known, it may be approximated by (Yalkowsky and Valvani, 1980):

$$\Delta S_f \sim 13.6 + 2.5\,(n - 5) \qquad (4.6)$$

where n is the number flexible atoms (i.e., atoms not involved in double bonds, triple bonds, or part of a ring structure) in the pollutant molecule, other than hydrogen. If n is less than 5, (n - 5) is set equal to zero.

---

*The original equations in the literature are different if they were reported in different solubility units. Refer to Section 4.2.2 for the appropriate solubility units conversion factors.

Correlation of K_{oc} and S_w is provided by (Kenaga and Goring, 1978):

$$\log K_{oc} = -0.55 \log S_w + 3.64 \qquad (4.7)$$

K_B can be correlated with K_{ow} by

$$K_B = 0.16\ K_{ow} \qquad (4.8)$$

4.2.2 Units and Conversion Factors

Three commonly used units of aqueous solubility are defined below:

(1) Mole fraction, x, the unitless ratio of the number of moles of solute to the total number of moles of solute plus water. In symbols, for a binary solution of n moles of solute in n_w moles of water

$$\begin{aligned} x &= n/(n + n_w) \\ &\sim n/n_w \text{ for } n_w >> n \end{aligned} \qquad (4.9)$$

(2) Molarity, S, expressed in moles of solute per liter of solution (M):

$$S(M) = n(\text{mol})/\text{liter of solution} \qquad (4.10)$$

(3) Weight fraction, expressed in milligrams of solute per liter of water, or parts per million, ppm

$$S_w\ (\text{ppm}) = \frac{n\ (\text{mol})\ MW\ (g\ \text{mol}^{-1})\ 1000\ (\text{mg}\ g^{-1})}{\text{liter of water}} \qquad (4.11)$$

where MW is the molecular weight of the solute.

For solutions with S < 1 M, one liter of aqueous solution contains approximately 55.5 moles of water. Thus

$$x = \frac{S}{55.5 + S} \sim \frac{S}{55.5} \text{ for } S < 1\ M \qquad (4.12)$$

or

$$S = \frac{55.5\ x}{(1 - x)} \sim 55.5\ x \text{ for } x < 10^{-2} \qquad (4.13)$$

To convert from molarity to ppm is straightforward by substituting Equation (4.10) into equation (4.11)

$$\text{ppm} \sim S(MW)\ (1000) \text{ for } S < 1\ M \qquad (4.14)$$

Thus to convert from mole fractions to ppm follows from equations (4.11) and (4.13)

$$\text{ppm} = \frac{55.5\ x}{(1 - x\ )}\ (MW)\ (1000)$$

$$\sim 55.5(x)\ (MW)\ (1000) \text{ for } x < 10^{-2} \qquad (4.15)$$

These conversion factors are summarized in Table 4.1.

Table 4.1

CONVERSION FACTORS FOR COMPOSITION UNITS

FROM \ TO	ppm	x (mole fraction)	M (Molarity)
ppm	---	$\frac{1.80 \times 10^{-5}}{MW}$	$\frac{10^{-3}}{MW}$
x (mole fraction)	5.55×10^{4} (MW)	---	55.5
M (Molarity)	(MW) (10^{3})	$\frac{1}{55.5}$	---

Concentration in aqueous solution is preferably given in mole fraction or molarity units since these units are measures of the amount of solute per amount of solution. The weight fraction or ppm, on the other hand, expresses the weight of solute per weight of solution and is thus a function of the molecular weight of the molecule, which is not relevant to environmental or toxicological effects.

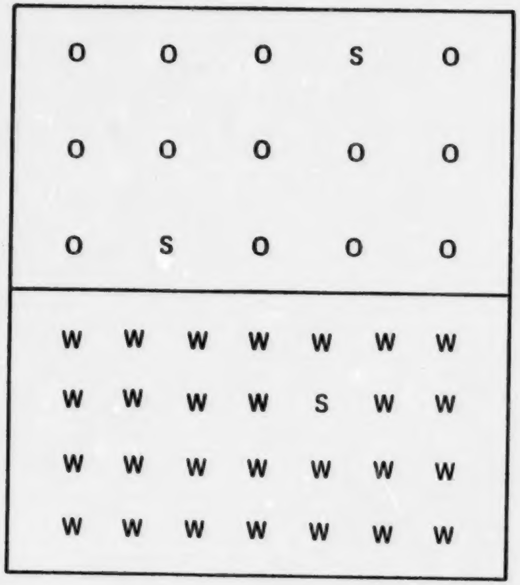
4.3 CALCULATION OF K_{oc} and S_w FROM K_{ow}

The sediment partition coefficient, normalized for organic carbon content (K_{oc}), and aqueous solubility (S_w) of an organic pollutant are critical to its environmental fate. Because K_{oc} and S_w values may be unmeasured or unreliable, it is important to be able to correlate these environmental parameters with other experimental quantitites, namely, to predict unmeasured values and appraise the reliability of measured values.

It is useful to correlate these parameters with octanol/water partition coefficients (K_{ow}) for practical as well as theoretical reasons. Practically, K_{ow} values are easier to measure and, where K_{ow} measurements have not been made, calculated values may be used with confidence. The theoretical basis for expecting correlations of K_{oc} and S_w with K_{ow} is described below. The correlation of K_B with other partitioning constants is not discussed in this section since a recent review of the subject is available.

4.3.1 Partitioning Thermodynamics

This discussion first considers the partitioning of a chemical between octanol and water, with octanol being a representative organic phase. If a small amount of a chemical is added to a closed vessel containing n-octanol and water, the vessel is shaken, and the octanol and water are allowed to separate, the chemical will partition between the two phases (see Figure 4.1). By convention, the small amount of chemical in each phase is called the solute. The partitioning of the solute molecules between the two phases can be understood in terms of a simple lattice model. If we assume that every molecule (water, octanol,


O O O S O
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O S O O O
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W W W W W W W

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FIGURE 4.1 LATTICE MODEL OF A SOLUTE (S) PARTITIONING BETWEEN OCTANOL (O) AND WATER (W) PHASES

$K_{ow} = C_o/C_w = 2$

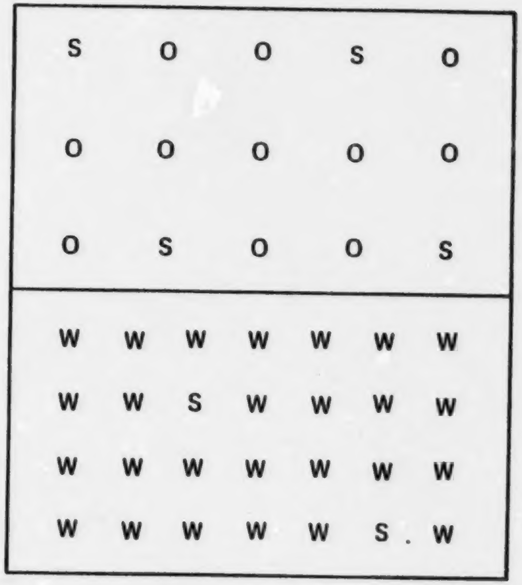
S O O S O
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FIGURE 4.2 LATTICE MODEL OF A HIGHER MOLE FRACTION OF SOLUTE (S) PARTITIONING BETWEEN OCTANOL (O) AND WATER (W) PHASES

Because the environment of each solute molecule is the same, $K_{ow} = C_o/C_w = 2$ as in Figure 4.1.

and solute) in both phases occupies a particular site on a three-dimensional lattice, with uniform spacing between sites, then the fraction of sites in each phase occupied by the chemical is the mole fraction x. A two-dimensional cross section of this lattice is shown in Figures 4.1 and 4.2.

The tendency for a solute molecule to leave either phase is proportional to the solute mole fraction in that phase and to the forces acting on the solute in that phase. The forces acting on a solute molecule will depend on which molecules occupy neighboring sites on the lattice. Figures 4.1 and 4.2 show that, over the mole fraction range of $x_w = 1/28$ to $x_w = 1/14$, solute molecules in the water phase are surrounded by water molecules. Thus, the forces acting on the solute in the water phase are independent of the solute mole fraction. Consequently, the tendency (f) of a solute molecule to leave the water phase is directly proportional to its mole fraction:

$$f = Hx \qquad (4.16)$$

where H is a constant representing the forces exerted on the solute by the solvent. At higher solute mole fractions, where solute-solute interactions become important (that is, where the solute is concentrated enough that solute molecules occupy neighboring lattice sites), H becomes a function [H(x)] of the solute mole fraction, and thus f is no longer directly proportional to x:

$$f = H(x)\, x \qquad (4.17)$$

The partitioning of the chemical between the octanol and water phases depends on this relative tendency of the chemical to leave each phase (f), which is conveniently viewed as a force per unit area. In thermodynamics, f is called the fugacity* and, as explained above, is proportional to the relative amount of the solute in the phase, x, and the forces acting on the solute within each phase; explicitly,

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*See, for example, G. L. Lewis and M. Randall, Thermodynamics, revised by K. S. Pitzer and L. Brewer (McGraw-Hill, NY, 1961).

$$f_w = (f^R \gamma_w)\ x_w \tag{4.18}$$

$$f_o = (f^R \gamma_o)\ x_o \tag{4.19}$$

where subscripts w and o refer, respectively, to the water and octanol phases, and f^R and γ_i are, respectively, the reference fugacity and activity coefficient, which together represent the forces acting on the solute in the i^{th} phase. At equilibrium

$$f_w = f_o \tag{4.20}$$

so that

$$x_o/x_w = \frac{f^R \gamma_w}{f^R \gamma_o} = \frac{\gamma_w}{\gamma_o} \tag{4.21}$$

In general, at constant pressure, f^R depends only on the temperature and γ_i depends on the composition as well as the temperature of the i^{th} phase. In sufficiently dilute solutions, however, the forces acting on a solute molecule will be independent of x_i because, as explained above, the environment of a solute molecule will remain constant. Thus $(f^R \gamma_i)$ will be a function only of temperature

$$(f^R \gamma_i) = H_i \tag{4.22}$$

where H_i is the Henry's constant for a very dilute solution of the solute in phase i. Thus

$$x_o/x_w = H_w/H_o \tag{4.23}$$

is a function only of temperature. However, if x_o or x_w is large enough that γ_o or γ_w is not constant, then K_{ow} will also no longer be constant.

Because composition is commonly measured in moles liter^{-1}(M), it is convenient to define:

$$K_{ow} = C_o/C_w = r_{wo}(x_o/x_w) = r_{wo}(H_w/H_o) \qquad (4.25)$$

where r_{wo} is a constant equal to the ratio of the molar volume of water

$$r_{wo} = v_w/v_o \quad (= 0.115) \qquad (4.26)$$

to that of octanol. (In terms of the lattice mode, r_{wo} is equal to the ratio of the number of sites per unit volume of octanol to that of water.)

Numerous workers have correlated the partitioning of chemicals between sediment and water and between biota and water with octanol/water partition coefficients. Before discussing these specific correlations in detail, it is useful to understand the conditions that must be met for these correlations to be successful.

Partitioning of a solute between water and any other water immiscible phase p (i.e., biota, sediment) may be described by

$$K_{pw} = r_{wp}(H_w/H_p) \qquad (4.27)$$

From equation (4.25) for partitioning between octanol and water

$$H_w = K_{ow}\,H_o/r_{wo} \qquad (4.28)$$

thus

$$K_{pw} = (r_{wp}/r_{wo})(H_o/H_p)K_{ow} = r_{op}(H_o/H_p)K_{ow} \qquad (4.29)$$

where r_{op} is the ratio of the molar volume of octanol to that of phase p. Thus, taking the logarithm of both sides of equation (4.29)

$$\log K_{pw} = \log K_{ow} + \log (r_{op}H_o/H_p) \qquad (4.30)$$

Thus, for the second term on the right-hand side of equation (4.30) to remain constant for a set of chemicals partitioning between water-octanol and water-phase p, phase p must be chemically similar to octanol and both K_{ow} and K_{pw} must be measured at low enough solute concentrations that solute-solute interactions are absent.

The success of K_{ow}-K_{oc} correlations (to be discussed in detail below), for example, may thus be understood. First, by normalizing adsorption for organic carbon content, we ensure the chemical similarity of phase p (that is, the organic content) and octanol. Second, the partitioning of the chemical between the water and sediment phases is usually measured at very low surface coverage (in the linear region of the adsorption isotherm) where adsorbate-adsorbate interactions are minimal.

Octanol/water partition coefficients have been used not only to correlate other partitioning data, but also to predict aqueous solubilities. The assumptions implicit in these predictions become apparent on close examination of the octanol/water partition experiment.

If it is assumed that the ratio of the number of solute molecules in each phase remains constant up to the limit of solubility, then

$$K_{ow} = (C_o/C_w)_{dilute} = (C_o/C_w)_{saturated} \qquad (4.31)$$

From equation (4.21), this means that the ratio of activity coefficients γ_w/γ_o remains constant up to saturation. As explained above, however, the ratio γ_x/γ_o will depend on solute concentration,* particularly if C_w (saturated) is large enough that solute-solute interactions become important. Furthermore, if we assume that the solubility of the chemical in pure water equals its solubility in the octanol-saturated water phase of the partition measurement, then

---

*Because of the chemical similarity of a neutral organic solute with n-octanol, it is expected that γ_o will not vary significantly with C_o.

$$K_{ow} = S_o/S_w \qquad (4.32)$$

where S_o and S_w are solubilities in moles liter^{-1}(M) in pure octanol and pure water, respectively.

To correlate aqueous solubility with K_{ow}, many authors have proposed an equation of the form:

$$\log S_w = -(1/a) \log K_{ow} + c \qquad (4.33)$$

where a and c are constants. Equation (4.33) may be derived by modifying equation (4.32) to account for deviations of real systems from model behavior:

$$K_{ow} = (S_o/S_w)^a \qquad (4.34)$$

This equation is clearly identical to equation (4.32) for $a = 1$. Taking the logarithm of both sides of equation (4.34) and rearranging terms:

$$\log S_w = - (1/a) \log K_{ow} + (1/a) \log S_o \qquad (4.35)$$

If S_o is assumed constant for a set of solutes in octanol, equation (4.35) becomes

$$\log S_w = - (1/a) \log K_{ow} + c \qquad (4.36)$$

and the correlation coefficients a and c may be calculated from a plot of known values of $\log S_w$ versus known values of $\log K_{ow}$ for the given set of solutes. Clearly, if the assumptions implicit in equation (4.32) are reasonable, the calculated value of a should be close to one.

The variability of S_o for a set of solutes is difficult to quantify except by comparing liquid and solid solutes. If two solutes are identical except that one is a liquid and the other is a solid in its pure state at temperature T, the solid will be less soluble than the liquid because of the additional energy required to remove solute molecules from the solid phase. Thus, if we assume that all liquid solutes have the same solubilities in n-octanol, and we use this pure liquid solute as the reference state, calculated solid solubilities must be corrected for the energy necessary to transform the solid to the liquid state. This energy is called the enthalpy of fusion, and from simple thermodynamic arguments, we can modify equation (4.35) for solid solutes:

$$\log S_w = -(1/a)\log K_{ow} + c - (1/a)\frac{\Delta H_f}{2.303\,RT_f}\ \frac{T_f - T}{T} \qquad (4.37)$$

where ΔH_f is the enthalpy of fusion, R is the gas constant, and T_f is the melting temperature of the solute. At the melting point,

$$\Delta H_f = T_f\,\Delta S_f \qquad (4.38)$$

Therefore at 25°C, equation (4.38) becomes

$$\log S_w = -(1/a)\log K_{ow} + c - \frac{\Delta S_f}{a(1360)}(\text{mp}-25) \qquad (4.39)$$

where mp is the melting point (in °C) and ΔS_f is the entropy of fusion (in cal deg^{-1} mole^{-1}). This correction is zero for solutes that are liquid at 25°C, but substantial for solutes with high melting points. Assuming that the theory is approximately correct and the correlation coefficient a is approximately equal to one, Table 4.2 and Figure 4.3 illustrate the magnitude of this correction as a function of melting point for a hypothetical solute with an uncorrected solubility of 100 ppm and a typical entropy of fusion of 13.6 entropy units (cal deg^{-1} mol^{-1}).

Table 4.2

EFFECT OF MELTING POINT CORRECTION ON WATER SOLUBILITY VALUES

Solubility (uncorrected) (ppm)	Melting Point (°C)	Solubility* (corrected) (ppm)
100	25	100
100	50	56
100	100	18
100	200	2
100	300	0.2

---

*$\log S_w$ (corrected) = $\log S_w$ (uncorrected) - 0.01 (mp-25) at 25°C, where $\Delta S_f = 13.6$ and $a = 1$ are assumed in equation (4.39) and S_w is the water solubility in ppm.

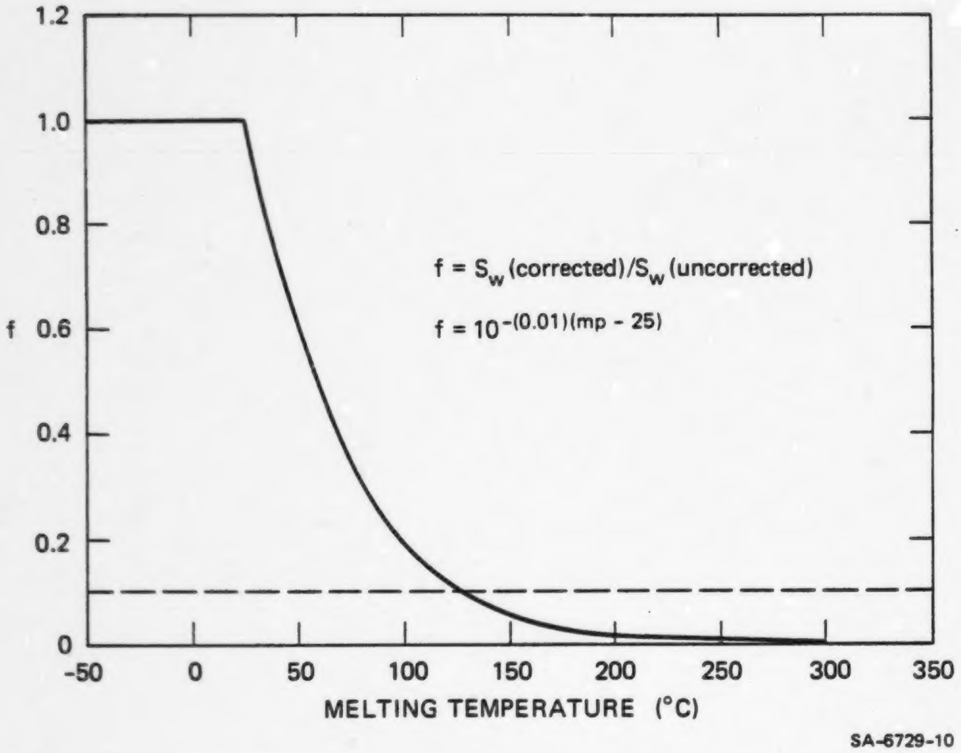

FIGURE 4.3 ENTHALPY OF FUSION CORRECTION FACTOR FOR AQUEOUS SOLUBILITY AT 25°C AS A FUNCTION OF MELTING TEMPERATURE

4.3.2 Comparison of Reported Correlations

Table 4.3 lists a representative sample of recently published correlations among K_{ow}, K_{oc}, S_w. This section examines these correlations in detail.

K_{oc}-K_{ow}. As discussed earlier, the sorption constant K_{oc} is the amount of chemical adsorbed per unit weight of organic carbon in the sediment divided by the equilibrium concentration of the chemical in the water phase. This constant is useful because, once K_{oc} has been determined for a chemical, the sorption partition coefficient may be calculated if the fraction organic content (f_{oc}) is known:

$$K_p = K_{oc}(f_{oc}) = C_s/C_w \tag{4.40}$$

where

K_p = Sorption partition coefficient

K_{oc} = Sorption partition coefficient normalized for organic carbon content

f_{oc} = Fraction of organic content in the sediment $(0 < OC < 1)$

C_s = Concentration of the adsorbed chemical

C_w = Equilibrium solution concentration.

Furthermore, it is useful to be able to predict K_{oc} values from the more easily measured K_{ow} values. The theoretical basis for expecting good K_{oc}-K_{ow} correlations has been discussed above. Two recent K_{oc}-K_{ow} correlations that have appeared in the literature are listed in Table 4.3. The significantly different correlation equations of Kenaga and Goring (1978) and Karickhoff et al. (1979) probably reflect the different data bases used to correlate K_{oc} with K_{ow}.

Table 4.3

REPORTED CORRELATIONS OF K_{ow}, K_{oc} AND S_w

Correlation	Equation	Eq.	Data Base*	Authors
$K_{oc} - K_{ow}$	$\log K_{oc} = 0.544 \log K_{ow} + 1.377$	(4.41)	Pollutants Aromatic hydrocarbons (8) Carboxylic acids and esters (5) Phosphorus containing insecticides (5) Ureas and uracils (7) Symmetrical triazines (6) Miscellaneous (14) Adsorbents Variety of soils	Kenaga and Goring (1978)
$K_{oc} - K_{ow}$	$\log K_{oc} = 1.00 \log K_{ow} - 0.21$	(4.3)	Pollutants Polycyclic aromatics (8) Chlorinated hydrocarbons (2)	Karickhoff et al. (1979)
$S_w - K_{ow}$	$\log S_w = -0.922 \log K_{ow} + 4.184$ S_w in ppm	(4.42)	Substituted benzenes and halobenzenes (12) Halogenated biphenyls and diphenyl oxides (11) Aromatic hydrocarbons (9) Phosphorus containing insecticides (16) Carboxylic acids and esters (9) Ureas and uracils (7) Miscellaneous (24)	Kenaga and Goring (1978)
$S_w - K_{ow}$	$\log x_s = -1.08 \log K_{ow} - 1.04 - \left[\frac{\Delta S_f}{1360} (mp - 25)\right]$	(4.43)	Simple aliphatics and aromatics in the following groups (n = 114) Alcohols Halogens Amines Carboxylic acids and esters Aldehydes and ketones Ethers Nitro compounds	Yalkowsky (1980)

x_s is the mole fraction solubility at 25°C

ΔS_f is the entropy of fusion in cal $\deg^{-1}$ mol^{-1}

mp is the melting point in °C (if mp $\leq$ 25 then the term in brackets is zero)

---

*Number in parentheses refer to the number of pollutants in the data base.

Table 4.3 (continued)

REPORTED CORRELATIONS OF K_{ow}, K_{oc} AND S_w

Correlation	Equation	Eq.	Data Base	Authors
$K_{oc} - S_w$	$\log K_{oc} = -0.55 \log S_w + 3.64$ in ppm	(4.7)	Similar to data base for equation (4.41)	Kenaga and Goring (1978)
$K_{oc} - S_w$*	$\log K_{om} = -0.56 \log S_w + 0.70$	(4.44)	Pollutants Polychlorinated biphenyls (3) Pesticides (4) Halogenated ethanes and propanes (6) Tetrachloroethene 1,2-Dichlorobenzene Adsorbents Willamette silt loam Miscellaneous other soils	Chiou et al. (1979)
	$\log K_{oc} = -0.56 \log S_w + 0.93$	(4.45)		
$K_{oc} - S_w$	$\log K_{oc} = -0.54 \log x_s + 0.44$ x_s in the mole fraction solubility	(4.46)	Similar to data base for equation (4.3)	Karickhoff (1979)

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*K_{om} is the sorption partition coefficient normalized for organic matter reported by Chiou et al. (1979). Assuming $K_a = 1.7\ K_{om}$, equation (4.45) is derived.

The theoretical equation of Table 4.4,

$$\log K_{oc} = 1.00 \log K_{ow} + \text{constant} \qquad (4.47)$$

follows from assuming that the second term on the right-hand side of equation (4.30) is constant; the data base required for a good fit with equation (4.47) follows from the assumptions used in the derivation of equation (4.30). It is clear from Table 4.4 that the data base and correlation equation of Karickhoff et al. (1979) closely conform with the theoretical model; however, the data base and correlation equation of Kenaga and Goring (1978) do not.

The advantages and disadvantages of using these alternative equations are not as well defined, however. Although the equation of Karickhoff et al. (1979) conforms to a simple model and accurately predicts sorption coefficients from K_{ow} data for a limited class of organic chemicals, it has not been widely tested and may be highly inaccurate for a more universal set of pollutants and soil/sediments. The equation of Kenaga and Goring (1978), however, is strictly empirical and only roughly predicts K_{oc} values from K_{ow} data, but it is applicable to a more universal set of pollutant/adsorbent systems because of the data base used. When more precise K_{oc} and K_{ow} data are available, it will be of interest to assess the predictive value of both of these correlations for both the universal set and individual classes of pollutant/adsorbent systems. It may become apparent that several correlation equations may be required to adequately predict K_{oc} values from K_{ow} values for the variety of systems of interest.

$\underline{S_w - K_{ow}}$. Several comparisons of the equations of Kenaga and Goring (1978) and Yalkowsky (1980) can be made. For reasons discussed earlier, the mole fraction units of solubility used by Yalkowsky are to be preferred to the ppm units used by Kenaga and Goring. In fact, to compare equation (4.42) of Kenaga and Goring with equation (4.43) of Yalkowsky, we must assume an average molecular weight for the chemicals in the data

Table 4.4

DATA BASES FOR K_{oc}-K_{ow} CORRELATIONS

	Kenaga and Goring (1978)	Karickhoff et al. (1979)	Theoretical
$\log K_{oc} =$	$0.54 \log K_{ow} + 1.38$	$1.00 \log K_{ow} - 0.21$	$1.00 \log K_{ow}$ + constant
K_{ow}	Measured and calculated values compiled from literature	Measured by Karickhoff et al.	Measured for very dilute solution
K_{oc}	Calculated average values for each chemical from adsorption coefficients for widely differing soils	Measured values for the silt (high organic content) fractions of two natural sediments	Uniform organic content of soil/sediment. Measured for adsorption from very dilute solutions
Chemicals	Very wide range of organic classes	Nonpolar or slightly polar organics	Nonpolar organics

base of Kenaga and Goring. Converting equation (4.42) from ppm to mole fractions units

$$\log x_s = -0.922 \log K_{ow} - 0.56 - \log MW \qquad (4.48)$$

where x_s is the mole fraction solubility and MW is the average molecular weight.

The variation of equation (4.48) with MW is shown in Figure 4.4 and compared with Yalkowsky's equation for liquid solutes. Two observations can be made about Figure 4.4. First, the molecular weight dependence of equation (4.48) is not very great for chemicals in the molecular weight range of 100-400. Second, because the average molecular weight of chemicals in the data base used to determine equation (4.48) is in the range of 100-400, it is clear that solubilities predicted by equation (4.48) will be approximately an order of magnitude lower than those predicted by equation (4.43).

A comparison of measured solubilities (in molarity units, M) with those predicted by the equations of Kenaga and Goring and of Yalkowsky is shown in Table 4.5 for a series of chlorinated methanes and ethanes. Note that all the chemicals listed in Table 4.5 (except hexachloroethane, which sublimes) are liquid at 25°C. Furthermore, is is clear from Table 4.5 that equation (4.43) of Yalkowsky predicts the aqueous solubility of chlorinated methanes and ethanes very accurately, whereas the corresponding prediction of equation (4.42) is an order of magnitude lower. Table 4.6, which compares calculated and measured solubilities for some low melting point aromatics, further supports these conclusions.

The cause of this discrepancy becomes clear when we examine the contrasting methods and data bases used by Kenaga and Goring and by Yalkowsky to develop their correlations. Kenaga and Goring empirically correlated K_{ow} with the solubility of a set of chemicals, most of which are solid at 25°C. In other words, Kenaga and Goring implicitly used a solid solute reference state; consequently, their correlation equation cannot accurately predict the solubility of a chemical that is liquid at 25°C.

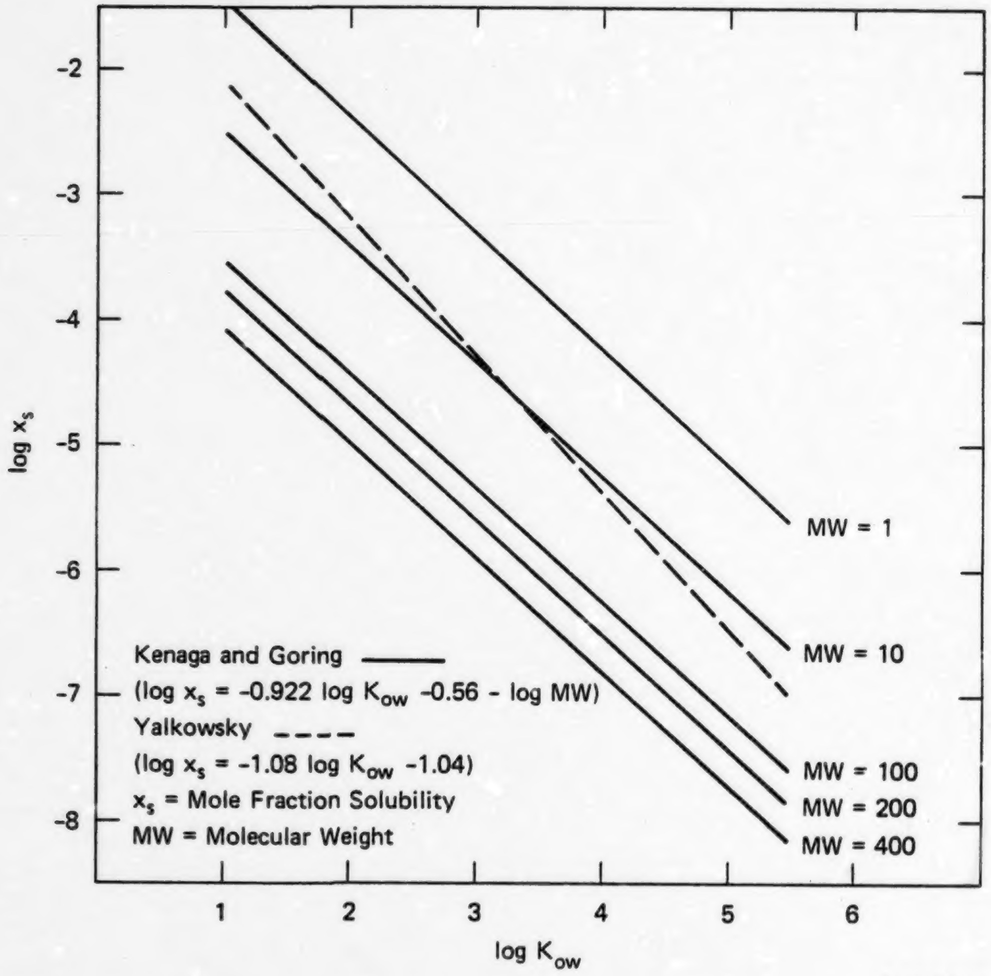

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FIGURE 4.4 COMPARISON OF SOLUBILITY - K_{ow} EQUATIONS FOR LIQUID SOLUTES

Table 4.5

CALCULATED VERSUS MEASURED SOLUBILITIES FOR CHLORINATED METHANES AND ETHANES

	log K_{ow}	mp (^oC)	log S_w (M) Kenaga and Goring	Yalkowsky	Measured
Chloromethane	0.95	-98	-1.4	-0.32	-0.89
Dichloromethane	1.26	-95	-1.87	-0.66	-0.80
Chloroethane	1.49	-136	-2.03	-0.91	-1.05
1,1-Dichloroethane	1.80	-97	-2.45	-1.24	-1.25
Trichloromethane	1.96	-64	-2.67	-1.41	-1.16
1,1.2-Trichloroethane	2.07	-37	-2.84	-1.53	-1.47
1,1,1-Trichloroethane	2.50	-30	-3.25	-2.00	-2.27
1,1,2,2-Tetrachloroethane	2.66	-36	-3.48	-2.17	-1.76
Tetrachloromethane	2.96	-23	-3.70	-2.49	-2.29
Hexachloroethane	4.62	Sublimes	-5.45	-4.29	-3.68

Yalkowsky, on the other hand, explicitly used a liquid solute reference state. To calculate the solubilities of chemicals that are solid at 25°C, Yalkowsky included an entropy of melting correction term. Thus the equation of Yalkowsky, assuming accurate known values of the entropy of fusion (ΔS_f) and melting point (T_f), is equally valid for liquid and solid solutes.

As discussed earlier, if two solutes are identical except that one is a liquid and the other is a solid in its pure state at 25°C, then the solid will be less soluble than the liquid by a factor of

$$\exp\left[-2.303(\Delta S_f/1360)(mp-25)\right] \qquad (4.49)$$

where ΔS_f is the entropy of fusion and mp is the melting point (°C). If ΔS_f is constant, then it is clear from equation (4.46) that solubility decreases as the melting point increases. Assuming $\Delta S_f = 13.6$ entropy units and converting mole fraction solubilities to molarity units, Figure 4.5 illustrates that equation (4.43) of Yalkowsky, in contrast with equation (4.42) of Kenaga and Goring, successfully predicts the decrease in solubility with increase in melting point for α-, β-, δ-, and γ-BHC.

Figure 4.5 also indicates that implicit in equation (4.42) of Kenaga and Goring is an empirical average of the solid solute correction term. Because the solubilities of liquid solutes predicted by equation (4.42) are approximately an order of magnitude lower than measured values, we can assume that this average correction term is approximately equal to 0.10, which is the dashed line in Figure 4.3. Thus, the predicted solubilities of equation (4.42) should approximate those of Yalkowsky and measured values for solutes with melting points in the 100° to 200°C temperature range. Figure 4.6 illustrates, in fact, that for solutes with an approximate molecular weight of 150, an entropy of fusion of 13.6 and a melting point of 125°C, the correlation equations of Yalkowsky and of Kenaga and Goring are similar. Moreover, Table 4.7 illustrates

Table 4.6

CALCULATED VERSUS MEASURED SOLUBILITIES FOR LOW MELTING POINT AROMATICS

		mp	log S_w (M)		
	log K_{ow}	(°C)	Kenaga and Goring	Yalkowsky	Measured
Nitrobenzene	1.87	5.6	-2.63	-1.32	-1.82
Benzene	2.13	5.5	-2.63	-1.60	-1.64
Toluene	2.79	-95	-3.35	-2.31	-2.24
Chlorobenzene	2.84	-45	-3.48	-2.37	-2.37
Ethylbenzene	3.34	-94.9	-3.92	-2.90	-2.85
1,2-Dichlorobenzene	3.56	-17	-4.26	-3.14	-3.00

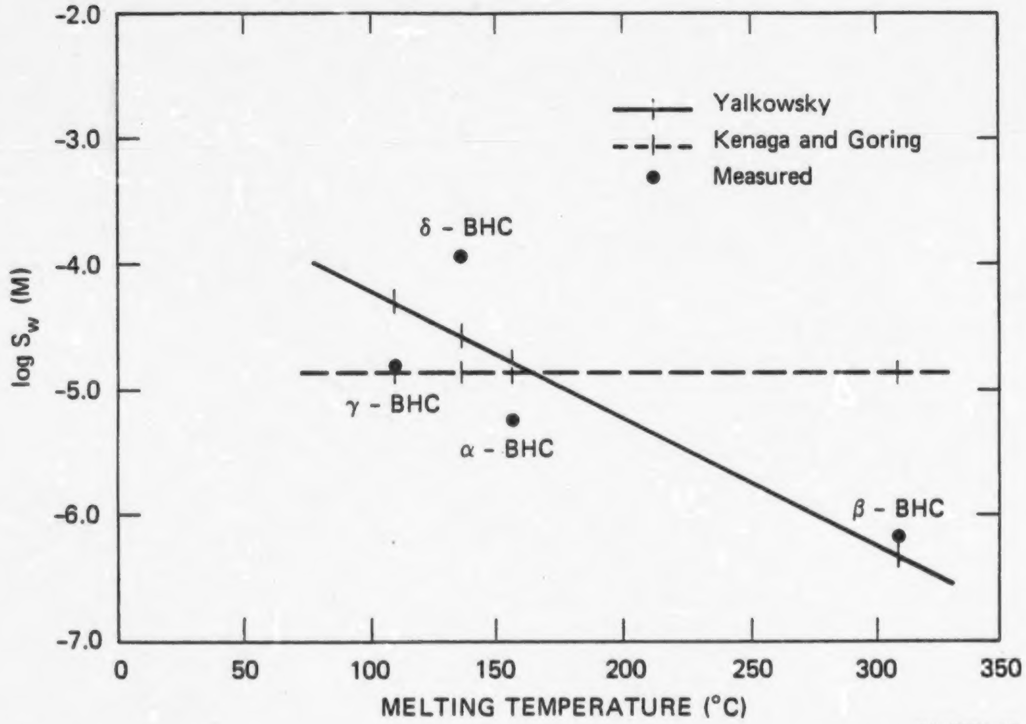

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FIGURE 4.5 SOLUBILITIES OF HEXACHLOROCYCLOHEXANES (α-, β-, δ-, γ-BHC) AS A FUNCTION OF MELTING TEMPERATURE

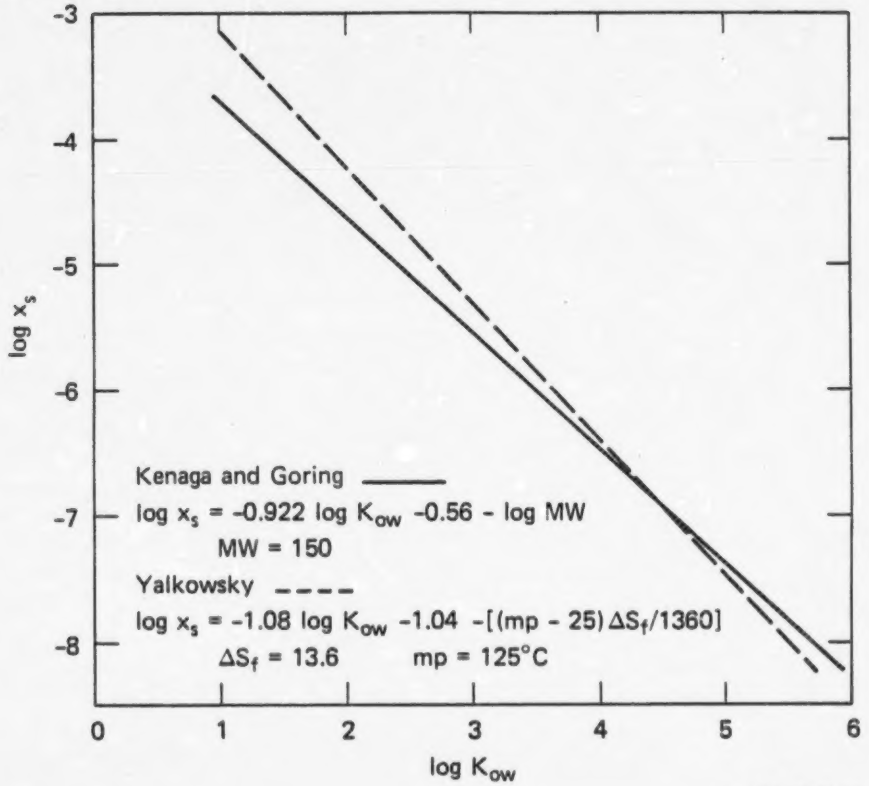

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FIGURE 4.6 COMPARISON OF SOLUBILITY - K_{ow} EQUATIONS FOR SOLID SOLUTES

Table 4.7

CALCULATED VERSUS MEASURED SOLUBILITIES FOR SELECTED PESTICIDES

	log K_{ow}	MP (^oC)	log S_w (M)		
			Kenaga and Goring	Yalkowsky	Measured
Lindane	3.89	113	-4.85	-4.38	-4.40 to -5.15
Aldrin	5.30	104	-6.24	-5.80	-6.30 to -7.35
Chlordane	5.48	108	-6.46	-6.04	-5.30 to -6.85
DDD	6.20	112	-7.04	-6.85	-6.5 to -7.2
DDT	6.91	109	-7.74	-7.59	-6.6 to -8.5

that for selected pesticides with melting points around 110°C the correlations of Yalkowsky and of Kenaga and Goring compare equally well with measured values.

Figure 4.5 also suggests that solubilities predicted from equation (4.42) of Kenaga and Goring will become progressively higher relative to measured values as the melting temperature increases above 200°C. Table 4.8 indicates that, indeed, measured solubilities of chemicals with melting points above 200°C systematically fall below those predicted by Kenaga and Goring.

In summary, equation (4.42) of Kenaga and Goring should be restricted to chemicals with melting points in the 100° to 200°C range, but equation (4.43) of Yalkowsky, because it includes a melting point correction factor is not limited by melting point restrictions.

$\underline{K_{oc} - S_w}$. To compare equation (4.7) with equations (4.45) and (4.46), it is again necessary to assume an average molecular weight for the correlation equation of Kenaga and Goring. If an average molecular weight of 200 is assumed, converting equations (4.7) and (4.45) to mole fraction solubility units gives

$$\log K_{oc} = -0.55 \log x_s - 0.23 \quad \text{(Kenaga and Goring, 1978)} \quad (4.50)$$

$$\log K_{oc} = -0.56 \log x_s - 0.04 \quad \text{(Chiou et al., 1979)} \quad (4.51)$$

$$\log K_{oc} = -0.54 \log x_s + 0.44 \quad \text{(Karickhoff et al., 1979)} \quad (4.46)$$

Several observations can be made about these equations. First, the similarity of equations (4.50) and (4.51) is remarkable, considering the contrasting data bases used by Kenaga and Goring and by Chiou et al. to determine their correlation coefficients. In fact, equations (4.50), (4.51), and (4.46) may all be written in the form

$$K_{oc} = (\text{constant})\ x_s^{-0.55(\pm 0.01)} \quad (4.52)$$

Table 4.8

AQUEOUS SOLUBILITIES OF HIGH MELTING POINT CHEMICALS

Chemical Name	Melting Point (^{o}C)	Solubilities (ppm) Measured	Solubilities (ppm) Predicted by Equation (4.42)[a]
Benzo[k]fluoranthene	217	5.6×10^{-4}	0.04
Anthracene	219	0.045	1.2
Benzo[g,h,i]perylene	222	2.6×10^{-4}	0.015
Chrysene	258	1.8×10^{-3}	0.1
Dibenz[a,h]anthracene	270	5×10^{-4}	9×10^{-3}
TCDD	303	2×10^{-4}	7.5×10^{-3}
B-BHC	309	0.24	4.0

---

[a] Kenaga and Goring (1978)

It is not clear why the solubility coefficient of -0.55(±0.01) should appear in each of these correlations. If as expected from the above discussions [see equations (4.3), (4.42), and (4.43)],

$$\log K_{oc} = a \log K_{ow} + \text{constant} \tag{4.53}$$

and

$$\log K_{ow} = - a \log x_s + \text{constant} \tag{4.54}$$

where $a \sim 1$, then by substituting equation (4.54) into equation (4.53)

$$\log K_{oc} = - a^2 \log x_s + \text{constant} \tag{4.55}$$

$$\sim - 1.0 \log x_s + \text{constant}$$

It is also apparent that none of these three equations accounts for the variation in solubility and hence variation in K_{oc} value with the melting point of the adsorbed chemical. The difference in adsorption behavior between solid and liquid solutes, in general, has been well documented in the literature (see, for example, Kipling, 1965). In fact, Roe (1975) has accounted for this difference in terms of the solid solute correction factor discussed earlier in this report. Karickhoff et al. (1979), in discussing their relatively poor correlation of K_{oc} with x_s (compared with their excellent correlation of K_{oc} with K_{ow}), mention that a correction term is probably needed in equation (4.40) to account for the enthalpy of fusion of the chemicals they studied.

$\underline{K_B - K_{ow}}$. The partitioning of organic chemicals has recently been reviewed by Baughman and Paris (1981), who noted the paucity of reliable data available for correlating K_B with other partitioning parameters. For the chemicals in Section 3, the following equation was used to calculate K_B

$$K_B = 0.16\ K_{ow} \tag{4.8}$$

which is the simplified version of the equation given by Baughman and Paris (1981),

$$\log K_B = 0.907 \log K_{ow} - 0.21 \qquad (4.56)$$

The reader is referred to the above review for an excellent exposition on the problems of reliably measuring K_B and the use of correlation equations to calculate K_B from S_w or from K_{oc} or K_{ow} data.

4.4 CALCULATION OF K_{ow} FROM STRUCTURAL PARAMETERS

The thermodynamics of partitioning of a chemical solution between octanol and water phases was discussed in 4.3.1, and the use of the octanol/water partition coefficient, K_{ow}, for calculating S_w, K_{oc} and K_B was described in Section 4.3.2. Although K_{ow} is the symbol used by many scientists for this partition coefficient, earlier literature and some current medical toxicology literature has commonly referred to the logarithm value of K_{ow} as "log P" (Hansch and Leo, 1979). For discussion in this section only, the log P nomenclature will be used instead of log K_{ow}, although the K_{ow} term will be used.

The K_{ow} data on the data sheets in Section 3 were calculated using a computer program developed at SRI; it uses the FRAGMENT method for calculating log P values (Hansch and Leo, 1979). The theory and procedures for these calculations are discussed in detail in that reference. Briefly, the method assumes that select groups of atoms in a molecule can be considered fragments, each of which contributes to the total log P value in an additive manner

$$\log P = \sum_{1}^{n} a_n f_n \qquad (4.57)$$

where a is the number of occurrences of fragment f of structural type n. Values of f have been empirically derived from the vast body of log P data available in the literature. Since the calculation of log P values for complex molecules can be time-consuming and subject to numerous calculation errors, the FRAGMENT calculation method and the data base for fragment values have been incorporated into a computer program using the PROPHET computer network.* The log P data are generated by first entering the structure on a graphic tablet. The log P program then uses an ordered substructure search routine to obtain fragment values for fragments of the molecular structure. Fragments are used, rather than atoms, because atomic contributions to log P vary with certain structural environments. The program then adds the fragment values to obtain log P values. It also identifies where the log P calculation may be incomplete because of the absence of values for particular fragments or because polar interactions must be accommodated by manual calculations. The log P program is under continuing development and evaluation at SRI and other laboratories.

The manual calculation of log P values using the FRAGMENT method is already established as a valid method for obtaining these data (Hansch and Leo, 1979). The calculations are, of course, subject to errors arising from subtle structural differences that are not recognized or cannot be accounted for when obtaining empirical values for the molecular fragments. In fact, the primary source of error is the original data on which the fragment values are based. The lack of reliable data is also a dilemma for verification of calculated log P values.

As an indicator of the accuracy of the log P calculation program Table 4.9 compares the K_{ow} values recently published by Hassett et al. (1980) with the K_{ow} values calculated by the log P program. Although the chemicals are not among the organic priority pollutants, they do represent some of the best K_{ow} data currently available. The calculated and measured K_{ow} values agree within the factor of two for 8 of the 14

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*PROPHET is a NIH resource available to biological and chemical scientists on a time-share basis. Information on the log P/PROPHET system can be obtained from Dr. Howard L. Johnson at SRI.

Table 4.9

CORRELATION OF MEASURED AND CALCULATED VALUES OF K_{ow}

Compound	Measured K_{ow} ± S.D.[a]	Computer-Calculated K_{ow}	Computer-Calculated r[b]
Pyrene	124,000 ± 11,000	79,400	1.6
7,12-Dimethylbenz[a]anthracene	953,000 ± 59,000	871,000	1.1
Dibenz[a,h]anthracene	3,170,000 ± 883,000	5,890,000	0.54
3-Methylcholanthrene	2,632,000 ± 701,000	9,330,000	0.28
Dibenzothiophene	24,000 ± 2,200	33,900	0.71
Acridine	4,200 ± 940	2,570	1.6
13H-Dibenzo[a,i]carbazole	2,514,000 ± 761,000	692,000	3.6
Acetophenone	38.6 ± 1.2	38.9	0.99
1-Napthol	700 ± 62	417	1.7
Benzidine	46.0 ± 2.2	35.5	1.3
2-Aminoanthracene	13,400 ± 930	1,660	8.1
6-Aminochrysene	96,600 ± 4,200	24,000	4.0
Anthracene-9-carboxylic acid	1,300 ± 130	15,500	0.08

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[a] Hassett et al. (1980).

[b] Ratio of measured K_{ow} to calculated K_{ow}.

compounds listed and agree within a factor of five for 12 of the 14 compounds. It is also significant to note that the last three compounds in Table 4.9 show the most disagreement between calculated and measured K_{ow} values, and these compounds are large molecules containing groups that may participate in H-bonding interactions.

In general, the accuracy of log P calculations by this method closely approaches the accuracy of experimental determinations performed over the last ten or twenty years because the fragment values were derived largely from those experimental data (by regression analysis) and incorporate the same experimental errors. It is not uncommon for measured log P values for a given compound in the literature to vary by 1 to 2 units; this corresponds to a factor of 10 to 100 in measured K_{ow} variation.

4.5 REFERENCES

Baughman, G. L., and D. F. Paris. 1981. Microbial Bioconcentration of Organic Pollutants from Aquatic Systems - A Critical Review. Critical Reviews in Microbiology, January 1981.

Chiou, C. T., L. J. Peters, and V. H. Freed. 1979. A Physical Concept Of Soil-Water Equilibria for Nonionic Organic Compounds. Science, 206, 831.

Hansch, C., and A. Leo. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology (Wiley-Interscience, New York)

Karickhoff, S. W., D. S. Brown, and J. A. Scott. 1979. Sorption of Hydrophobic Pollutants on Natural Sediments. Water Research 13, 241.

Kenaga, E. E., and C. A. I. Goring. 1978. Relationship Between Water Solubility. Soil-Sorption, Octanol-Water Partitioning and Bioconcentration of Chemicals in Biota. ASTM, Third Aquatic Toxicology Symposium, October 17-18, New Orleans, LA

Kipling, J. J. 1965. "Adsorption From Solutions of Non-Electrolytes", (Academic Press, London).

Lewis, G. L., and M. Randall. 1961. "Thermodynamics", revised by K. S. Pitzer and L. Brewer, (McGraw-Hill, New York).

Roe, R. J. 1975. Adsorption of Solid Solutes from Solution: Application of the Multilayer Theory of Adsorption. J. Colloid Interface Sci., 50, 64.

Yalkowsky, S. H. and S. C. Valvani. 1980. Solubility and Partitioning I: Solubility of Nonelectrolytes in Water. J. Pharm. Sci., 69, 912.